

Quantum statistical theory of dislocation mobility in discrete lattices

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We present a first-principles quantum statistical theory of dislocation motion based on discrete lattice dynamics and the Keldysh nonequilibrium formalism. By treating the dislocation as a moving source coupled to the phonon field through exact Kanzaki forces, we derive a universal memory kernel that captures all phononmediated dissipation mechanisms without adjustable parameters. The theory naturally produces the experimentally observed drag regimes: linear phonon wind at low velocities, quadratic radiation damping at intermediate speeds, and finite drag enhancement near the speed of sound. Crucially, we demonstrate that the elastodynamic prediction of an infinite sound barrier is an artefact of continuum approximations; the discrete lattice structure and anharmonic phonon interactions regularize all singularities, permitting transonic motion at finite stress. Through systematic reduction via conserving approximations, we obtain practical mobility laws suitable for crystal plasticity and dislocation dynamics simulations. These take the form of either steady state algebraic relations or minimal differential systems that capture memory effects while adding negligible computational cost. All parameters derive directly from harmonic and anharmonic force constants, enabling predictive modeling across ten orders of magnitude in strain rate. Application to fcc and bcc metals yields drag coefficients and relaxation times in good agreement with molecular dynamics and available experiments, validating the approach. This work establishes a microscopic foundation for dislocation mobility and provides a pathway from atomistic properties to continuum plasticity without empirical fitting.

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I. INTRODUCTION

This work concerns the mobility of crystalline dislocations at the atomistic scale. Dislocation mobility is arguably the most important aspect underpinning crystal plasticity [1]. Indeed, Orowan's equation [2], $\dot{\gamma} = B\bar{v}\rho_m$, an exact average of the collective effect of dislocations in a crystal, shows that for a given dislocation ensemble of Burgers vector B , the plastic strain rate $\dot{\gamma}$ is proportional to the average glide velocity $\bar{v}$ and the mobile dislocation density ρ_m . Because dislocation density varies slowly in most conventional plastic deformation events [1,3], it is the ensemble-averaged glide velocity of dislocations that most often explains the rate at which crystalline solids accommodate permanent deformation. Thus any constitutive model of strength, rate sensitivity, or strain hardening (Ref. [3]) must rest on a faithful representation of the underlying mobility law that mediates dislocation motion.

Dislocation mobility is usually framed in terms of describing $\bar{v}$ in relation to external stimuli acting on the dislocation, such as temperature T and applied stress τ . How to do so remains a challenge. While the glide of individual dislocations can be resolved at the mesoscale [4], and the collective behavior of the microstructure inferred macroscopically [5], the motion itself is conditioned by the atomistic structure of the dislocation core and its interaction with the lattice, with

external driving forces, and with other microstructural defects. The range of physical mechanisms proposed to influence mobility, including so-called lattice resistance [6], phonon and electron scattering [7–11], inertial and radiative damping [12–15], and solute drag [16], amongst many others, has led to mobility laws expressed in the very general, very vague form of $v_d = f(\tau, \dots)$, relating the glide velocity v_d to an applied resolved shear stress τ and whatever other effects need be included. This expression encodes the assumption that dislocations dissipate the energy gained from applied loads through a variety of microscopic processes, all of which contribute to an effective drag force opposing their motion.

The theoretical quest to derive dislocation mobility from first principles has a rich history spanning over seven decades. The foundational work of Eshelby [17–19] in the 1950s established the equations of motion for dislocations and introduced concepts of radiation effects from moving dislocations, though within the limitations of continuum elasticity. Concurrently, Nabarro's development of the Peierls-Nabarro model [6,20] provided a semidiscrete approach to understanding lattice friction, bridging atomistic and continuum descriptions. The “phonon wind” theory by Leibfried and collaborators [21,22] in the 1950s–1960s described how moving dislocations scatter thermal phonons, yielding the classical result of drag proportional to temperature in the high-temperature, low-velocity limit [6,7,21].

Alshits and Indenbom [10] developed a systematic quantum-mechanical framework for computing drag coefficients, though still restricted to low velocities and simplified phonon spectra. More recently, Blaschke and collaborators [11,14] extended this phonon wind theory to include full

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velocity dependence up to transonic speeds and incorporated crystallographic anisotropy effects, providing semi-analytic expressions for drag in various crystal systems. Their approach revealed the importance of crystal geometry in determining velocity-dependent drag but relied on simplified Debye phonon spectra and continuum approximations for the dislocation field. Perhaps the most radical recent development is the quantized “dislon” theory by Li, *et al.* [23], which treats dislocations as quantum field excitations analogous to phonons. This approach enables calculation of quantum many-body effects and electron-phonon-dislocation interactions from first principles, though its application to mobility calculations remains in early stages.

Despite these theoretical advances, a unified framework that simultaneously captures lattice discreteness, quantum statistics, anharmonic effects, and arbitrary velocities within a single consistent formalism remains elusive. Existing approaches typically excel in certain regimes while requiring phenomenological extensions or failing entirely in others. Continuum theories diverge at sound speeds, phonon wind models neglect anharmonicity and core structure, molecular dynamics (MD) provides only observational data without general laws, and even sophisticated quantum approaches have yet to yield practical mobility expressions for engineering applications. This theoretical fragmentation has practical consequences: crystal plasticity and dislocation dynamics simulations must rely on empirical mobility laws with limited transferability across temperature and strain rate regimes.

Broadly speaking, three regimes of dislocation motion are usually identified [3,16]. At the lowest end of the applied stress range lies the *activation of motion* regime, concerned with describing the physics of dislocation lines under the action of stresses below the Peierls barrier [1]. Remarkable research has focused on describing the physics behind this problem, in which the dislocation is believed to hop stochastically over the Peierls barrier through the kink-pair mechanism [24–26]. This work is not concerned with this regime, whose description requires a toolkit other than that developed here. Once the barrier is overcome, dislocations are believed to enter the so-called “free glide” or *viscous drag* regime, thus called because the dislocation is seemingly subject to a viscous-like drag force whereby $v_d \propto \tau$. Theoretical studies across continuum, atomistic, and lattice-dynamical frameworks have proposed a broad range of mechanisms for this dislocation drag, including phonon and electron viscosities [22,27,28], radiative damping [17–19,29–31], thermoelastic coupling [30,32,33], and solute interactions [34–36], each contributing competing physical interpretations and mathematical forms for the stress–velocity relation. These formulations remain either incompatible with one another or valid only in restricted regimes of speed, temperature, or dislocation character. Finally, at the higher end of applied stress ranges, dislocations are believed to enter the *inertial regime*, thus called because linear elasticity predicts the appearance of a sound barrier that on the one hand prevents dislocations from achieving trans- and supersonic speeds, and on the other entails an increased amount of energy dissipation through acoustic damping. Indeed, inertial contributions derived from radiative self-energies, whether via quasirelativistic expressions [1,29,37] or more sophisticated

time-dependent formulations in the elastodynamic continuum [15,38–41], produce divergent or transient predictions near the sound speeds, which have since been posited to act as a “barrier” to dislocation motion [17], whether surmountable or not. However, because these models rely on the elastodynamic continuum’s foundational assumptions, they can only aim to capture acceleration rates, not viscous glide, and are physically limited by the underlying constraints posed by the elastic continuum, which is nondispersive and nondiscrete, unlike the local environment of a dislocation. In turn, phonon scattering models, whether analytic or semiphenomenological [10,11,15,42], likewise depend critically on the choice of steady state elastic fields and lattice dispersion relations, often inducing drag divergences at or below c_t .

The theoretical uncertainties concerning dislocation mobility are compounded by experimental limitations, particularly in the inertial regime. Indeed, direct tracking of dislocations at high velocities remains technically infeasible: etch-pit chronometry [43], slip-band growth [21,44], acoustic attenuation, and even the most advanced *in-situ* electron microscopy provide reliable data only up to dislocation speeds of order $c_t/3$ [45]. Above this threshold, all available evidence is indirect or inferred from bulk response. Certain macroscopic phenomena, such as thermal hardening observed in a multitude of metals under high strain rate deformation [46–49], suggest the operation of a viscous-like phonon drag proportional to dislocation velocity and temperature [50,51]. Others, such as magnetoplastic effects [52,53] or anomalous yield maxima in superconducting states [54], implicate weak electronic dissipation or radiative inertia. Yet even when experimental datasets exist, the fitted mobility exponents vary widely [26], from thermally activated sublinear scaling to abrupt transonic transitions, with little mechanistic consensus [3,55,56].

Atomistic simulation, typically performed via MD, although capable of resolving core structure and phonon emission without phenomenological input, introduces its own ambiguities. Chiefly, the observational nature of MD simulations prevents the enunciation of a general mobility law, instead limiting such modeling attempts to phenomenological fits of extracted data points (e.g., Refs. [57–61]); in effect, MD mobility laws extend experimental efforts at mobility reconstruction. Further, results vary significantly with potential choice, simulation cell geometry, loading method, and boundary conditions, and mobility plateaus or velocity jumps frequently depend on artificial resonance effects or discretization artefacts [59–63]. Supersonic motion, first observed in tungsten [62] and later in other metals [64,65], confirmed the kinematic possibility of such motion but failed to yield a universal transferable stress–velocity law: the terminal stress values and velocity discontinuities depend sensitively on the glide plane geometry and simulation setup, to the point that recent models show observed velocity plateaus around the sound barrier (see, e.g., Ref. [62]) to be caused by the resonance of the dislocation’s own acoustic fields with the inevitable hard boundaries that simulation cell setups require [66,67]. Thus even MD simulations introduce artefacts into the study of dislocation mobility. Nevertheless, they largely align with conclusions from harmonic lattice dynamics [63,68,69], where discreteness and dispersion regularize

the divergence at c_t , suggesting that continuum singularities and sound barriers are not physical invariants but artefacts of idealized elasticity.

This fragmentary evidence appears to stem from a conceptual impasse. On the one hand, it is clear that across all crystalline solids, dislocation mobility is not governed by a universal, closed-form law of the type $v_d = f(\tau)$, nor can it be reliably predicted by phenomenological regressions extrapolated beyond their calibration range [58,70,71]. On the other hand, dislocation dynamics simulations, crystal plasticity models, and in general, constitutive laws for use in engineering practice, all demand such input, lest they remain untethered to microscale kinetics. The central problem is therefore not merely one of parameter estimation, but of formulating a physically consistent, microscopically grounded theory that connects lattice-scale dissipation to observable glide behavior across the subsonic, transonic and supersonic regimes.

It is precisely this theoretical gap that the present work seeks to address. After outlining the basis of a formal harmonic lattice model of a crystalline lattice in Sec. II. In Sec. III, we exploit it to deduce a 0 K, phononinduced mobility law. We then extend this framework to account for thermal effects and anharmonicities in a self-consistent description of dislocation drag. In Sec. IV, we develop a conserving Keldysh field [72] formulation for dislocation-phonon interactions, augmented by our deterministic Kanzaki forces [73,74] and respecting the gauge invariance of the crystalline lattice. With this, we provide a field theoretic basis for dislocation mobility that transcends both the limitations of ad hoc regularization and the assumptions of linear drag. Our construction admits anharmonic corrections, which we introduce in Sec. V, incorporating into it the stochastic phonon backreaction. This leads to a complete, quantum thermal anharmonic framework of dislocation mobility whose sole missing component is that of electronic effects not captured through the atomic interactions. As we show, the formulation reproduces lattice viscosity and radiative damping in a single unified framework that, as we discuss in Sec. VII, avoids spurious divergences at sound speeds and requires no phenomenological insertion of core dissipation. By doing so, we aim to reconcile simulation, theory and observation, and furnish a predictive, physically principled foundation for low, moderate, and high speed dislocation mobility laws, whose practical extraction for dislocation dynamics and CPFE simulations we describe in Sec. VIII. Section IX closes the article by outlining the main findings and the way forward.

II. DISCRETE LATTICE DYNAMICS AND KANZAKI FORCE REPRESENTATION

We first establish the fundamental framework for treating dislocation motion in discrete crystalline lattices. We begin by constructing the harmonic lattice dynamics on a finite Born-von Kármán supercell [75]. We then introduce the discrete Kanzaki force representation that captures the topological nature of dislocations through bond-level slip fields, which we will employ in the sequel.

Throughout this work, we denote the mass density by ρ , the Lamé parameters by μ and λ , the transverse and longitudinal

sound speeds by c_T and c_L respectively, and the magnitude of the Burgers vector by B (with $\mathbf{B}$ denoting the vector).

A. Discrete harmonic lattice framework

Consider a Bravais lattice $\Lambda = \{\mathbf{R}_n = n_a \boldsymbol{\alpha}_a \mid n_a \in \mathbb{Z}\}$ with primitive vectors $\boldsymbol{\alpha}_a \in \mathbb{R}^3$ and unit cell volume $V = \boldsymbol{\alpha}_1 \cdot (\boldsymbol{\alpha}_2 \times \boldsymbol{\alpha}_3)$. To render the system computationally tractable while preserving the essential physics, we impose Born-von Kármán periodic boundary conditions that repeat the lattice after N_a cells along each primitive direction. This gives the finite direct lattice

$$\Lambda^p = \{\mathbf{R}_n \mid 0 \leq n_a < N_a\}, \quad |\Lambda^p| = N \equiv N_1 N_2 N_3. \quad (1)$$

The reciprocal lattice construction follows naturally. The dual basis vectors $\mathbf{b}_a \in \mathbb{R}^3$ satisfy the orthogonality condition $\mathbf{b}_a \cdot \boldsymbol{\alpha}_b = 2\pi \delta_{ab}$, ensuring that plane waves $e^{i\mathbf{k} \cdot \mathbf{R}}$ with wave vectors

$$\mathbf{k}_\kappa = \frac{\kappa_a}{N_a} \mathbf{b}_a, \quad \kappa_a = 0, 1, \dots, N_a - 1, \quad (2)$$

are commensurate with the periodic boundary conditions. The allowed wave vectors form a discrete three-torus $\mathcal{T}$ of cardinality N , which serves as the reciprocal space for all subsequent Fourier analysis.

Discrete Fourier transform pair. The finite lattice admits a natural discrete Fourier transform that preserves all symmetries of the crystalline system. For any function $f : \Lambda^p \rightarrow \mathbb{C}$, we define the transform pair

$$\tilde{f}(\mathbf{k}_\kappa) = \frac{1}{N} \sum_{\mathbf{R} \in \Lambda^p} f(\mathbf{R}) e^{-i\mathbf{k}_\kappa \cdot \mathbf{R}}, \quad (3)$$

$$f(\mathbf{R}_n) = \sum_{\mathbf{k}_\kappa \in \mathcal{T}} \tilde{f}(\mathbf{k}_\kappa) e^{i\mathbf{k}_\kappa \cdot \mathbf{R}_n}. \quad (4)$$

The inversion formula follows from the orthogonality of discrete exponentials on the torus, which ensures that

$$\sum_{\mathbf{R} \in \Lambda^p} e^{i(\mathbf{k}_\kappa - \mathbf{k}_{\kappa'}) \cdot \mathbf{R}} = N \delta_{\kappa, \kappa'}. \quad (5)$$

This discrete transform naturally incorporates the finite size of real crystals and automatically provides the ultraviolet cutoff that regularizes all physical quantities.

Harmonic lattice Hamiltonian. The starting point for lattice dynamics is the displacement vector $\mathbf{u}(\mathbf{r}, t) \in \mathbb{R}^3$ of an atom at lattice site $\mathbf{r} \in \Lambda^p$ from its perfect-lattice position. Under the harmonic approximation, which captures the essential physics of phonon propagation and linear elasticity [76], the total energy separates into kinetic and potential contributions:

$$H = \frac{1}{2} \sum_{\mathbf{r}} \frac{|\mathbf{p}(\mathbf{r})|^2}{m(\mathbf{r})} + \frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}'} \sum_{i,j} u_i(\mathbf{r}, t) \Phi_{ij}(\mathbf{r} - \mathbf{r}') u_j(\mathbf{r}', t), \quad (6)$$

where $\mathbf{p}(\mathbf{r}) = m(\mathbf{r}) \dot{\mathbf{u}}(\mathbf{r})$ is the canonical momentum, $u_i(\mathbf{r}, t)$ denotes the i -th Cartesian component of the displacement at site $\mathbf{r}$, and $\Phi_{ij}(\mathbf{R}) \in \mathbb{R}$ is the (i, j) component of the force-constant matrix coupling atoms separated by lattice vector $\mathbf{R}$.

The harmonic approximation is physically well-justified for small-amplitude vibrations and enables exact solution

of the lattice dynamics problem [63,68,77–79]. The force-constant matrix inherits the translational symmetry of the underlying crystal, depending only on the separation $\mathbf{r} - \mathbf{r}'$ rather than absolute positions. This symmetry, combined with momentum and angular momentum conservation, imposes the sum rules:

$$\sum_{\mathbf{R}} \Phi_{ij}(\mathbf{R}) = 0 \quad (\text{translational invariance}), \quad (7)$$

$$\sum_{\mathbf{R}} [\Phi_{ik}(\mathbf{R})R_j - \Phi_{jk}(\mathbf{R})R_i] = 0 \quad (\text{rotational invariance}). \quad (8)$$

These identities ensure that uniform translations and rotations of the entire crystal produce no net internal forces, thereby preserving the fundamental symmetries in the discrete setting.

Mass-weighted coordinates and the dynamical matrix. To diagonalize the equations of motion, we introduce mass-weighted displacements that equalize the inertial weight of each degree of freedom. For a monatomic lattice with mass m , the Fourier-transformed displacement field is $\tilde{u}_i(\mathbf{k}, t) = \sqrt{m} \sum_{\mathbf{r}} u_i(\mathbf{r}, t) e^{-i\mathbf{k} \cdot \mathbf{r}}$, and the dynamical matrix becomes

$$D_{ij}(\mathbf{k}) = \frac{1}{m} \tilde{\Phi}_{ij}(\mathbf{k}), \quad (9)$$

where $\tilde{\Phi}_{ij}(\mathbf{k}) = \sum_{\mathbf{R} \in \Lambda^p} \Phi_{ij}(\mathbf{R}) e^{-i\mathbf{k} \cdot \mathbf{R}}$ is the Fourier-transformed force-constant matrix. The dynamical matrix is Hermitian for all $\mathbf{k} \in \mathcal{T}$.

The eigenvalue problem for the dynamical matrix,

$$\sum_j D_{ij}(\mathbf{k}) e_{j,\alpha}(\mathbf{k}) = \omega_{\alpha}^2(\mathbf{k}) e_{i,\alpha}(\mathbf{k}), \quad (10)$$

determines the phonon frequencies $\omega_{\alpha}(\mathbf{k})$ and their corresponding polarization vectors $\mathbf{e}_{\alpha}(\mathbf{k})$, where $\alpha = 1, 2, 3$ labels the phonon branches. The orthonormality condition $\sum_i e_{i,\alpha}^*(\mathbf{k}) e_{i,\beta}(\mathbf{k}) = \delta_{\alpha\beta}$ ensures completeness: $\sum_{\alpha} e_{i,\alpha}(\mathbf{k}) e_{j,\alpha}^*(\mathbf{k}) = \delta_{ij}$, enabling any lattice field to be expanded in these normal coordinates.

Equations of motion and lattice Green function. In Fourier space, the mass-weighted displacements $\tilde{u}_i(\mathbf{k}, t)$ satisfy the equation of motion [80]

$$\ddot{\tilde{u}}_i(\mathbf{k}, t) = - \sum_j D_{ij}(\mathbf{k}) \tilde{u}_j(\mathbf{k}, t). \quad (11)$$

Each eigenvector $\mathbf{e}_{\alpha}(\mathbf{k})$ oscillates independently with frequency $\omega_{\alpha}(\mathbf{k})$, reducing the coupled problem to a collection of uncoupled harmonic oscillators.

The lattice Green function, i.e., the frequency domain resolvent of the equations of motion, is defined in terms of the force-constant matrix as [80]

$$G_{ij}(\mathbf{k}, \omega) = \frac{1}{m} [\omega^2 \delta_{ij} - D_{ij}(\mathbf{k})]^{-1} = \frac{1}{m\omega^2 \delta_{ij} - \tilde{\Phi}_{ij}(\mathbf{k})}. \quad (12)$$

This object plays a central role in our subsequent analysis: it propagates unit body forces at frequency ω and encodes the complete linear response of the harmonic lattice. The Green function is analytic off the real frequency axis and satisfies Kramers-Kronig relations, reflecting the causal structure of lattice dynamics [81].

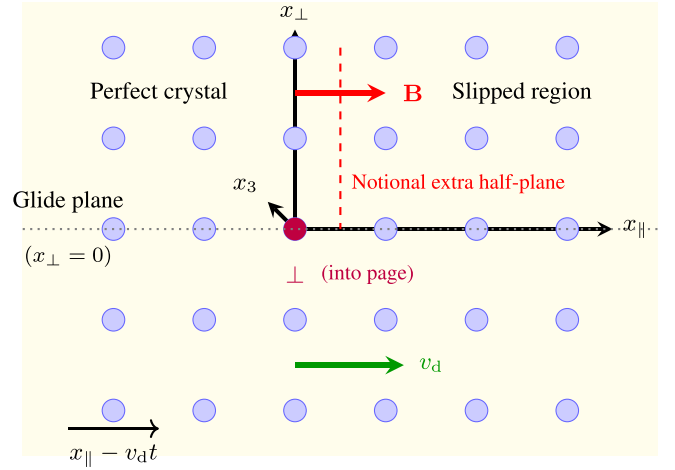


FIG. 1. Two-dimensional view of an edge dislocation in the glide plane. The coordinate system has $x_{\parallel}$ as the glide direction, $x_{\perp}$ normal to the glide plane, and x_3 along the dislocation line (perpendicular to the page). The dislocation core is marked by $\perp$, with the extra half-plane of atoms (dashed red line) terminating at the core. The Burgers vector $\mathbf{B}$ and glide velocity v_d are both parallel to $x_{\parallel}$. For a screw dislocation, the Burgers vector would be parallel to x_3 .

A crucial feature of the discrete lattice Green function is its exponential decay in real space when the force constants have finite range. This short-range character confines all non-locality to a radius of a few lattice constants, while long-range effects are carried by the smooth phonon dispersion $\omega_{\alpha}(\mathbf{k})$. This separation of scales [82] proves essential for constructing well-behaved dislocation mobility kernels free of low frequency divergences.

B. Kanzaki force representation for gliding dislocations

Having established the harmonic lattice framework, we now construct the discrete Kanzaki force representation that describes a uniformly gliding dislocation in a perfect harmonic lattice. The Kanzaki force approach, originally derived for the modeling of point defects in the harmonic lattice [83–85], has been extended to other crystal defects [73,74], and captures the topological nature of dislocations through the fundamental discontinuity in the displacement field, while remaining fully consistent with the discrete lattice structure.

We work in Cartesian coordinates $\mathbf{r} = (x_{\parallel}, x_{\perp}, x_3)$ where as shown in Fig. 1, the dislocation line coincides with the x_3 axis, the glide direction is $x_{\parallel}$, and $x_{\perp}$ lies in the glide plane. The dislocation translates rigidly at speed v_d along $x_{\parallel}$, ensuring that all fields depend only on the Galilean-invariant combination $x_{\parallel} - v_d t$.

Bond level slip representation. Rather than attempting to describe dislocation glide through a site-based displacement field we employ a bond-level description that naturally incorporates the topological discontinuity [63,68,73]. We introduce a slip indicator function $\Psi(\mathbf{r}, \mathbf{r}')$ that equals $+1$ if the bond connecting lattice site $\mathbf{r}'$ to site $\mathbf{r}$ crosses the glide plane from below to above, -1 if it crosses from above to below, and zero otherwise.

This bond indicator approach correctly localizes the Burgers discontinuity on the discrete set of bonds intersected by

the moving slip interface, avoiding the artificial smearing inherent in continuum treatments. For a glide plane at $x_{\perp} = 0$ translating at constant speed v_d , the imposed rigid displacement is

$$u_j(\mathbf{r}, t) = B_j \Theta(x_{\parallel} - v_d t), \quad (13)$$

where $\mathbf{B} = (B_j)$ is the Burgers vector and Θ denotes the Heaviside function. This defines a piecewise-uniform displacement field whose discontinuity is physically realized through the orientation of slip-carrying bonds.

Discrete Kanzaki force construction. The key insight of the Kanzaki method is that any prescribed displacement field can be realized in the harmonic lattice through an equivalent distribution of body forces [83]. As shown in [73], convolving the displacement field Eq. (13) with the harmonic force-constant matrix yields the slip contribution to the total Kanzaki force:

$$F_i^{\text{slip}}(\mathbf{r}, t) = - \sum_{j, \mathbf{r}'} B_j \Phi_{ij}(\mathbf{r} - \mathbf{r}') \Psi(\mathbf{r}, \mathbf{r}') \Theta(x'_{\parallel} - v_d t). \quad (14)$$

The antisymmetry of the slip indicator $\Psi(\mathbf{r}, \mathbf{r}') = -\Psi(\mathbf{r}', \mathbf{r})$ combined with the symmetry of the force-constant matrix $\Phi_{ij}(\mathbf{r} - \mathbf{r}') = \Phi_{ji}(\mathbf{r}' - \mathbf{r})$ automatically ensures conservation of total force and torque:

$$\sum_{\mathbf{r}} F_i^{\text{slip}}(\mathbf{r}, t) = 0, \quad (15)$$

$$\sum_{\mathbf{r}} \epsilon_{ijk} r_j F_k^{\text{slip}}(\mathbf{r}, t) = 0. \quad (16)$$

This force distribution reproduces the classical Volterra elastic field at large distances from the dislocation while maintaining exact force balance.

Core corrections and multipole representation. The slip representation Eq. (14) models the dislocation as an infinitely sharp cut, neglecting the discrete core structure. In reality, the core extends over several lattice spacings and exhibits significant departures from linear elasticity. These effects can be systematically incorporated through a localized core correction [74]:

$$F_i^{\text{core}}(\mathbf{r}, t) = F_i^{\text{total}}(\mathbf{r}, t) - F_i^{\text{slip}}(\mathbf{r}, t), \quad (17)$$

where F_i^{total} represents the complete force distribution required to generate the actual dislocation structure; it can be calculated from atomistic simulations of dislocations, as shown in [74].

For our purposes, we note that the core contribution is exponentially localized on the scale of the Burgers vector magnitude and admits a systematic multipole expansion [74,86], detailed in Appendix A. For our purposes, it suffices to retain only the leading dipole term, which captures the dominant elastic moment generated by the discrete core structure. In Fourier space, this corresponds to:

$$\tilde{F}_i^{\text{core}}(\mathbf{k}, \omega) \simeq ik_j \tilde{M}_{ij}(\omega) + \mathcal{O}(k^2), \quad (18)$$

where $\tilde{M}_{ij}(\omega)$ is the time-Fourier transform of the dipole moment tensor. Higher-order moments may be included to refine short-wavelength behavior but remain negligible in the long-wavelength limit relevant for radiative processes.

Fourier space representation and radiative response. For dynamical calculations, it proves convenient to work in frequency-momentum space. The Fourier transform of the slip contribution Eq. (14) yields (see Appendix B):

$$\tilde{F}_i^{\text{slip}}(\mathbf{k}, \omega) = - \sum_j \Phi_{ij}(\mathbf{k}) B_j \tilde{\Psi}(\mathbf{k}) \frac{(2\pi)\delta(\omega - v_d k_{\parallel})}{k_{\parallel} + i0^+}, \quad (19)$$

where the pole structure $1/(k_{\parallel} + i0^+)$ arises naturally from the Fourier transform of the Heaviside function and encodes the proper causal prescription. In the sequel, we drop the $\sum_j$ term for brevity, and leave the summation implicit.

The total lattice response to this driving force is obtained through convolution with the lattice Green function:

$$\tilde{u}_i(\mathbf{k}, \omega) = G_{ij}(\mathbf{k}, \omega) \tilde{F}_j(\mathbf{k}, \omega), \quad (20)$$

$$G_{ij}(\mathbf{k}, \omega) = [\rho \omega^2 \delta_{ij} - \Phi_{ij}(\mathbf{k})]^{-1}, \quad (21)$$

where ρ is the mass density and $D_{ij}(\mathbf{k})$ is the dynamical matrix Eq. (9).

This construction provides a complete, self-consistent description of dislocation motion in discrete lattices. The slip contribution dominates the infrared (long-wavelength) response and recovers classical elasticity in appropriate limits, while the core corrections capture ultraviolet physics and ensure proper regularization of all observables. The Fourier representation (19) forms the foundation for all subsequent calculations of phonon radiation and mobility, naturally incorporating both the topological character of dislocations and the discrete structure of crystalline matter.

A key advantage of the discrete approach is that all integrals over the Brillouin zone are automatically finite. The bounded domain $|\mathbf{k}| \leq \pi/a$ provides a natural high-frequency cutoff that eliminates the logarithmic and power-law divergences that plague continuum elastodynamic theories. This regularization is not artificial: it reflects the genuine discrete structure of crystalline matter and ensures that all physical observables remain finite and well-defined.

Despite this, the framework smoothly recovers all known continuum results in appropriate limits [76]. For wavelengths much longer than the lattice spacing, $|\mathbf{k}| \ll a^{-1}$, the dynamical matrix reduces to its isotropic elastic form and the discrete Kanzaki forces reproduce the classical Burridge-Knopoff [87] force representation, and through them, the eigenstrain frameworks used in micromechanics [88].

Thus this framework provides the foundation for constructing quantum-statistical mobility laws that unify all velocity regimes, from quasistatic creep through viscous drag to radiation-limited high speed motion, within a single analytic structure free of empirical parameters or artificial regularizations.

III. ZERO-TEMPERATURE MOBILITY IN THE FULLY DISCRETE LATTICE

At absolute zero, a uniformly gliding dislocation still radiates phonons, because the time-dependent *discrete* Kanzaki forces act as a parametric drive on the harmonic crystal. We derive here the exact lattice-level mobility functional and then obtain the familiar $P \propto v^5/\tau \propto v^4$ law by an explicit

long-wavelength expansion that keeps every lattice constant explicit and introduces *no* phenomenological core width.

A. Exact radiated power

With $\tilde{F}_j(\mathbf{k}, \omega)$ the total Kanzaki spectrum of a line moving at speed v_d (Eq. (19)) and the lattice Green's function $G_{ij}(\mathbf{k}, \omega) = [\rho\omega^2\delta_{ij} - \Phi_{ij}(\mathbf{k})]^{-1}$, the power per unit line length is

$$P[v_d] = \frac{1}{2} \sum_{\alpha=1}^3 \int_{\text{BZ}} \frac{d^3k}{(2\pi)^3} \omega_{\alpha}(\mathbf{k}) |e_{i,\alpha}(\mathbf{k}) G_{ij}(\mathbf{k}, \omega_{\alpha}) \times \tilde{F}_j(\mathbf{k}, \omega_{\alpha})|^2 (2\pi) \delta[\omega_{\alpha}(\mathbf{k}) - v_d k_{\parallel}]. \quad (22)$$

where $\alpha = 1, 2, 3$ indexes of the phonon polarization branches, with corresponding eigenfrequencies $\omega_{\alpha}(\mathbf{k})$ and polarization vectors $e_{i,\alpha}(\mathbf{k})$ obtained from the diagonalization of the dynamical matrix $D_{ij}(\mathbf{k}) = \rho^{-1} \Phi_{ij}(\mathbf{k})$.

Let τ be the resolved shear stress acting on the dislocation, driving its motion with velocity v_d . The energy balance for a segment of Burgers magnitude B then defines the *exact* mobility functional yields

$$\tau[v_d] = \frac{P[v_d]}{B v_d}, \quad (23)$$

which is valid for any crystal symmetry and all velocities v_d . Direct evaluation of Eq. (23) can be computationally demanding, as the radiated power functional $P[v_d]$ requires integration over the full Brillouin zone's Doppler surface and involves summation across all phonon branches. Careful inspection of the integrand, however, reveals that significant analytical simplifications are possible without sacrificing accuracy or physical insight. Specifically, the slip projector $(\delta_{ij} - \hat{k}_i \hat{k}_j)$ constrains the Kanzaki force components that couple effectively to the phonon field: for a screw dislocation, it entirely removes any component parallel to $\hat{\mathbf{k}}$, so that only *transverse acoustic* modes contribute. In contrast, for an edge dislocation, the Kanzaki force retains a finite longitudinal component along the wavevector, thus coupling to both transverse and longitudinal acoustic branches. Nonetheless, pseudo-optic replicas resulting from zone-folding effects remain excluded, carrying zero spectral weight in either case. Moreover, along the glide direction $\mathbf{k} = k_{\parallel} \hat{x}_{\parallel}$, the delta functions $\delta(k_{\perp})\delta(k_3)$ collapse the three-dimensional integral to a straightforward one-dimensional Doppler condition. Because the acoustic dispersion is strictly linear ($\omega_{\alpha} = c_{\alpha}|k_{\parallel}|$) along this reduced integral path, the resulting principal-value integral remains analytically tractable and finite. In the sequel, we detail some of simplifications, particularly in the account of thermal effects given in Sec. IV.

B. Scaling and asymptotic behavior on the small-k limit

Before tackling Eq. (23) directly, we examine the asymptotic behavior of the physics it entails. For a glide dislocation, the *slip* component of the Kanzaki spectrum (core multipoles only renormalize higher orders) is, from Eq. (19),

$$\tilde{F}_j(\mathbf{k}, \omega) = -\frac{\Phi_{j\ell}(\mathbf{k}) B_{\ell} \tilde{\Psi}(\mathbf{k})}{k_{\parallel} + i0^+} (2\pi) \delta(\omega - v_d k_{\parallel}), \quad (24)$$

where $\tilde{\Psi}$ is the lattice Fourier transform of the bond slip indicator introduced in Sec. II B. Note that for brevity, we leave the summation term implied.

For $|\mathbf{k}| \ll a^{-1}$, two controlled expansions are required. First, the force constant matrix takes its isotropic-elastic form

$$\Phi_{j\ell}(\mathbf{k}) = \mu k^2 (\delta_{j\ell} - \hat{k}_j \hat{k}_{\ell}) + (\lambda + \mu) k_j k_{\ell} + \mathcal{O}(k^4),$$

while the indicator reduces to the continuum jump distribution

$$\tilde{\Psi}(\mathbf{k}) \xrightarrow{|\mathbf{k}| \ll a^{-1}} i\pi (2\pi)^2 \delta(k_{\perp}) \delta(k_3) \text{sgn } k_{\parallel}.$$

Because rotational invariance forbids an $\mathcal{O}(k)$ anisotropic correction, the next nonvanishing term for the jump appears at $\mathcal{O}(k^3)$.

Using the identity

$$\frac{\text{sgn}(k_{\parallel})}{k_{\parallel} + i0^+} = \frac{1}{|k_{\parallel}|} - i\pi \delta(k_{\parallel}),$$

and neglecting the nonradiative $\delta(k_{\parallel})$ term, the Fourier transform of the transverse Kanzaki force on the acoustic shell $\omega = c_T k$ becomes

$$\begin{aligned} \tilde{F}_j^{(T)}(\mathbf{k}, \omega) &= -i\pi \mu B k^2 \frac{(\delta_{jm} - \hat{k}_j \hat{k}_m) \hat{B}_m}{|k_{\parallel}|} (2\pi)^2 \delta(k_{\perp}) \delta(k_3) \\ &\times (2\pi) \delta(\omega - v_d k_{\parallel}), \end{aligned} \quad (25)$$

where $\hat{\mathbf{k}} = \mathbf{k}/|\mathbf{k}|$, and no artificial smearing or regularization is invoked; the spectrum follows from lattice elasticity alone.

To compute the radiated power, we contract Eq. (25) with the transverse Green function [88]

$$G_{ij}^{(T)}(\mathbf{k}) = -\frac{\delta_{ij} - \hat{k}_i \hat{k}_j}{\rho c_T^2 k^2},$$

and form the modulus squared of the projected force, as required in the spectral power formula:

$$\begin{aligned} |e_{i,T}(\mathbf{k}) G_{ij}^{(T)}(\mathbf{k}) \tilde{F}_j^{(T)}(\mathbf{k}, \omega)|^2 \\ = \frac{\mu^2 B^2}{\rho^2 c_T^4} \frac{[(\delta_{pq} - \hat{k}_p \hat{k}_q) \hat{B}_q]^2}{k_{\parallel}^2} (2\pi)^4 \delta^2(k_{\perp}) \delta^2(k_3). \end{aligned} \quad (26)$$

Longitudinal polarizations do not contribute at this order since $e_{i,L} \parallel \hat{\mathbf{k}}$.

Substituting Eq. (26) into the discrete spectral formula and performing the $\mathbf{k}$ integral using the delta functions yields a one-dimensional Doppler integral along the direction of motion:

$$\begin{aligned} \int_{-\pi/a}^{\pi/a} \frac{dk_{\parallel}}{k_{\parallel}^2} \delta(c_T |k_{\parallel}| - v_d k_{\parallel}) \\ = \frac{2(v_d/c_T)^2}{c_T \sqrt{1 - (v_d/c_T)^2}} \text{P} \int_0^{k_{\max}} \frac{dk}{k^3}, \end{aligned}$$

where $k_{\max} = \pi/a$ marks the Brillouin zone boundary. The integrand is even under $k_{\parallel} \mapsto -k_{\parallel}$, and the principal value integral remains finite due to lattice regularization. No ultraviolet divergence arises.

The geometric factor $[(\delta_{pq} - \hat{k}_p \hat{k}_q) \hat{B}_q]^2$ distinguishes screw and edge dislocations. The delta functions constrain the wave

vector to $\mathbf{k} = k_{\parallel} \hat{x}_{\parallel}$, implying $\hat{k}_3 = 0$. For a screw dislocation, $\hat{\mathbf{B}} \parallel x_3$, so $\hat{B}_q = \delta_{q3}$, and the projector simplifies to δ_{p3} , yielding

$$\mathcal{A}_{\text{screw}} = 1.$$

For an edge dislocation, where $\hat{\mathbf{B}}$ lies in the $x_{\parallel}$ - $x_{\perp}$ plane, an azimuthal average over $\hat{\mathbf{B}} = (\cos \phi, \sin \phi, 0)$ and $\hat{\mathbf{k}} = (\cos \theta, \sin \theta, 0)$ gives

$$\mathcal{A}_{\text{edge}} = \frac{3}{4}.$$

Collecting all prefactors, the universal zero-temperature radiated power becomes

$$P[v_d] = \frac{\mu B^2}{24\pi \rho c_T^2} \mathcal{A} v_d^3, \quad \mathcal{A} = \begin{cases} 1, & \text{screw,} \\ \frac{3}{4}, & \text{edge.} \end{cases} \quad (27)$$

Balancing the power $P = \tau B v_d$ with the work done yields the corrected mobility relation

$$\tau(v_d) = \frac{\mu}{24\pi} \frac{\mathcal{A}}{\rho c_T^2} \frac{v_d^2}{B}, \quad v_d \ll c_T. \quad (28)$$

We must remark that longitudinal contributions are suppressed by a factor k^2 , entering only at $O(v_d^4)$, and core multipoles affect only numerical prefactors via $O(k^0)$ corrections, without altering the scaling. Finally, in the continuum limit $a \rightarrow 0$, the principal value integral vanishes, recovering the classical result that a steady Volterra dislocation in linear elasticity does not radiate [18].

Equation (28) is therefore the fully discrete, parameter-free zero-temperature mobility law underpinning all subsequent quantum-thermal generalizations. Remarkably, the quadratic drag law of Eq. (28) coincides with Nabarro's original scaling estimate for a gliding Volterra line [6]. The same v^2 dependence emerges from Hart's calculation of the elastic energy emitted by a vibrating dislocation [89], and from the power radiated by a kink train in the Frenkel-Kontorova model [6], suggesting that seemingly disparate microscopic pictures converge on an identical velocity scaling laws. The agreement, however, is no accident: each of those disparate models can be obtained as a limiting case of the present Kanzaki-Green's function framework, so they must reproduce the same infrared exponent. In all instances, the drag coefficient is generated solely by the kinematic coupling between the dislocation's slip field and transverse acoustic modes; with no adjustable parameters and no ultraviolet divergence, its functional form is dictated completely by the lattice symmetry, the $1/k_{\parallel}$ structure of the Kanzaki force, and the geometry of the Doppler shell.

IV. QUANTUM-THERMAL DYNAMICS OF THE GLIDING DISLOCATION

Dislocation motion at nonzero temperature couples the lattice to a moving source that exchanges energy not only with the vacuum (zero-point) phonon field, but also with thermal excitations already present in the crystal. This interaction alters both the energy radiated by the dislocation and the resulting mobility law. Whereas the zero-temperature calculation in Sec. III involved only spontaneous phonon emission, finite temperature enables stimulated emission and absorption

processes. A full quantum-statistical treatment is therefore essential to capture the temperature dependence of the dislocation's drag force.

To describe this energy exchange correctly, here we treat the dislocation as a classical source moving through a quantum harmonic lattice. We will model the lattice degrees of freedom as a thermalized bosonic environment (i.e., a quantum many-body bath) characterized by phonon operators obeying Bose-Einstein statistics [90,91]. Importantly, the phonon response is not instantaneous, so the energy exchange is inherently nonlocal in time, even when the dislocation trajectory is uniform and deterministic.

An appropriate framework for such quantum-statistical dynamics out of equilibrium is the Schwinger-Keldysh closed time path formalism [72,92], which allows causal evaluation of observables in the presence of a time-dependent external source [92]. It is well suited to calculating expectation values in a system subject to both quantum and thermal fluctuations, as it encodes not only the response (via the retarded Green function) but also the statistical correlations (via the Keldysh component).

In what follows, we compute the radiated power and resulting mobility law using this framework, taking as input the corrected Kanzaki force spectrum derived in Sec. II B, which properly accounts for the lattice discreteness and the dislocation's slip topology without resorting to artificial core regularization or continuum elasticity. This approach enables an exact and consistent treatment of phononmediated dissipation in the quantum-thermal regime.

A. Thermal phonon correlations and deterministic dislocation forcing

Our starting point is the standard harmonic lattice Hamiltonian $H_0 = \frac{1}{2} \sum_{\mathbf{r}} p_i(\mathbf{r})^2/m + \frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}'} u_i(\mathbf{r}) \Phi_{ij}(\mathbf{r} - \mathbf{r}') u_j(\mathbf{r}')$, where $u_i(\mathbf{r})$ denotes atomic displacements and $\Phi_{ij}(\mathbf{R})$ is the force constant matrix. Diagonalization via normal modes yields $u_i(\mathbf{k}, t) = \sum_{\alpha} e_{i,\alpha}(\mathbf{k}) Q_{\alpha}(\mathbf{k}, t)$, where $e_{i,\alpha}(\mathbf{k})$ are, again, the polarization vectors and Q_{α} are the canonical phonon coordinates with frequencies $\omega_{\alpha}(\mathbf{k})$.

In thermal equilibrium at temperature T , we assume that each mode is populated according to the Bose distribution [90]

$$n_B(\omega) = \frac{1}{\exp(\hbar\omega/k_B T) - 1}. \quad (29)$$

In the Keldysh formalism, correlation functions are organized into a 2×2 matrix structure with contour indices $a, b \in \{+, -\}$ representing the forward and backward branches of the closed-time contour. For free phonons in thermal equilibrium, the Green's function components are well-established [72]. The retarded and advanced functions take the form

$$G_{\alpha}^{\text{R/A}}(\mathbf{k}, \omega) = \frac{1/\rho}{\omega^2 - \omega_{\alpha}^2(\mathbf{k}) \pm i0^+}, \quad (30)$$

while the Keldysh component reads

$$G_{\alpha}^{\text{K}}(\mathbf{k}, \omega) = -2\pi i \coth\left(\frac{\hbar\omega}{2k_B T}\right) \text{sgn } \omega \delta(\omega^2 - \omega_{\alpha}^2(\mathbf{k})), \quad (31)$$

These satisfy the fluctuation-dissipation relation $G^K = \coth(\hbar\omega/2k_B T)(G^R - G^A)$, where the thermal factor $\coth(\hbar\omega/2k_B T) = 2n_B(\omega) + 1$ encodes both stimulated processes (proportional to n_B) and spontaneous emission (the $+1$ term) [72].

Now we introduce a straight dislocation gliding at constant velocity v_d along the slip direction $x_{\parallel}$, following the trajectory $X(t) = v_d t$. The dislocation exerts a force on the lattice atoms given by the Kanzaki force density, whose Fourier transform is given in Eq. (24). The key point to note here is that this force is purely classical: it has no operator character and no quantum fluctuations. The interaction Hamiltonian thus takes the form

$$H_{\text{int}}(t) = \sum_{\mathbf{k}, j} \tilde{F}_j(\mathbf{k}) u_j(\mathbf{k}, t) e^{ik_{\parallel} v_d t}, \quad (32)$$

where the phase factor $e^{ik_{\parallel} v_d t}$ arises from the moving source, with $k_{\parallel}$ being the component of $\mathbf{k}$ along the glide direction.

The classical nature of the dislocation source has important consequences for its representation on the Keldysh contour. A classical field couples identically to both branches, which we encode in the contour coupling matrix

$$\sigma^{ab} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad a, b \in \{+, -\}. \quad (33)$$

This structure ensures that the diagonal components vanish ($\tilde{F}^{++} = \tilde{F}^{--} = 0$) while the off-diagonal components are equal ($\tilde{F}^{+-} = \tilde{F}^{-+} = \tilde{F}$), reflecting the fact that a classical source generates no intrinsic fluctuations.

To compute the phonon self-energy, we project the interaction onto normal modes. This defines the coupling vertex

$$V_{\alpha}(\mathbf{k}) = \frac{e_{j,\alpha}(\mathbf{k}) \Phi_{j\ell}(\mathbf{k}) B_{\ell} \tilde{\Psi}(\mathbf{k})}{\sqrt{2\rho\omega_{\alpha}(\mathbf{k})} (k_{\parallel} + i0^+)}, \quad (34)$$

where B_{ℓ} is the Burgers vector and $\tilde{\Psi}(\mathbf{k})$ contains the geometric factors specific to the dislocation configuration. The normalization ensures that $|V_{\alpha}(\mathbf{k})|^2$ is dimensionless, as appropriate for a vertex in the path integral formulation. Crucially, we do not impose energy conservation at this stage, as it will emerge naturally from the dynamics.

In the harmonic formalism (i.e., to second order in perturbation theory), the self-energy involves the time-ordered correlation of two interaction vertices. On the Keldysh contour, this yields

$$\Sigma_{\alpha}^{ab}(\mathbf{k}, \omega) = \frac{i}{\hbar^2} |V_{\alpha}(\mathbf{k})|^2 \sigma^{ab} \int_{-\infty}^{\infty} dt e^{i(\omega - v_d k_{\parallel})t}. \quad (35)$$

The time integral produces the energy-conserving delta function:

$$\int dt e^{i(\omega - v_d k_{\parallel})t} = 2\pi \hbar \delta(\omega - v_d k_{\parallel}). \quad (36)$$

Thus we obtain

$$\Sigma_{\alpha}^{ab}(\mathbf{k}, \omega) = i |V_{\alpha}(\mathbf{k})|^2 2\pi \delta(\omega - v_d k_{\parallel}) \sigma^{ab}. \quad (37)$$

Given the structure of σ^{ab} , the off-diagonal components are

$$\Sigma_{\alpha}^{+-} = \Sigma_{\alpha}^{-+} = i |V_{\alpha}(\mathbf{k})|^2 2\pi \delta(\omega - v_d k_{\parallel}),$$

while the diagonal components vanish: $\Sigma_{\alpha}^{++} = \Sigma_{\alpha}^{--} = 0$.

The retarded and advanced self-energies, defined as $\Sigma^R = \Sigma^{++} - \Sigma^{+-}$ and $\Sigma^A = \Sigma^{++} - \Sigma^{-+}$, also vanish for a classical source. This reflects the fact that a classical driving force does not renormalize the phonon frequencies, but rather it merely induces transitions between existing states.

The physically relevant quantity is the Keldysh self-energy

$$\Sigma^K = \Sigma^{+-} + \Sigma^{-+} = 2i |V_{\alpha}(\mathbf{k})|^2 2\pi \delta(\omega - v_d k_{\parallel}).$$

However, this expression corresponds to driving a zero-temperature system. To incorporate thermal effects, we must account for the fact that the dislocation interacts not with bare phonons but with a thermal bath.

In thermal equilibrium, phonon propagators carry the statistical factor $F(\omega) = \coth(\hbar\omega/2k_B T) = 2n_B(\omega) + 1$ [90,91]. When the classical dislocation couples to the thermal phonon bath, each phonon line in the self-energy diagram contributes this thermal weight. Since the Keldysh self-energy involves summing the $+-$ and $-+$ contractions, each containing one thermal phonon propagator, the full result is dressed by the same Bose factor:

$$\Sigma_{\alpha}^K(\mathbf{k}, \omega) = 2i |V_{\alpha}(\mathbf{k})|^2 [2n_B(\omega) + 1] 2\pi \delta(\omega - v_d k_{\parallel}). \quad (38)$$

This final expression Eq. (38) captures the complete physics of phonon emission from a gliding dislocation in a thermal crystal.

Within the Debye approximation, where $\omega_{\alpha}(\mathbf{k}) = c_{\alpha} |\mathbf{k}|$ with sound velocity c_{α} , we can evaluate the phase-space integral explicitly. The resonance condition $c_{\alpha} |\mathbf{k}| = v_d k_{\parallel} = v_d k \cos \theta$ restricts the wavevector magnitude to

$$k = \frac{v_d \cos \theta}{c_{\alpha}}, \quad (39)$$

where θ is the angle between $\mathbf{k}$ and the glide direction. This is only possible for $\cos \theta \geq v_d/c_{\alpha}$, requiring $v_d < c_{\alpha}$ for real solutions.

In spherical coordinates with polar axis along $\hat{\mathbf{e}}_{\parallel}$, the delta function integral becomes:

$$\begin{aligned} & \int d^3k \delta(c_{\alpha} k - v_d k \cos \theta) \\ &= \int_0^{k_D} k^2 dk \int_0^{\pi} \sin \theta d\theta \int_0^{2\pi} d\phi \delta(c_{\alpha} k - v_d k \cos \theta). \end{aligned} \quad (40)$$

The delta function can be rewritten as

$$\begin{aligned} \delta(c_{\alpha} k - v_d k \cos \theta) &= \frac{1}{k} \delta\left(\frac{c_{\alpha} - v_d \cos \theta}{v_d}\right) \\ &= \frac{1}{v_d k \sin \theta} \delta(\theta - \theta_c), \end{aligned} \quad (41)$$

where $\theta_c = \arccos(v_d/c_{\alpha})$ is the cone angle. Performing the angular integrals:

$$\int_0^{\pi} \sin \theta d\theta \frac{1}{v_d k \sin \theta} \delta(\theta - \theta_c) = \frac{1}{v_d k} \quad (42)$$

and the azimuthal integral gives 2π . The radial integral with the constraint $k = v_d \cos \theta / c_{\alpha}$ yields

$$\int d^3k \delta(c_{\alpha} k - v_d k_{\parallel}) = \frac{2\pi}{v_d c_{\alpha}^2} \int_0^{\theta_c} \frac{v_d^2 \cos^2 \theta}{c_{\alpha}^2} \sin \theta d\theta. \quad (43)$$

Evaluating this integral:

$$\int_0^{\theta_c} \cos^2 \theta \sin \theta d\theta = \left[-\frac{\cos^3 \theta}{3} \right]_0^{\theta_c} = \frac{1}{3}(1 - \cos^3 \theta_c) \quad (44)$$

$$= \frac{1}{3} \left[1 - \left(\frac{v_d}{c_\alpha} \right)^3 \right]. \quad (45)$$

However, the power integral involves not just the phase space but also the vertex factor $|V_\alpha(\mathbf{k})|^2 \propto k^2/(k^2 + \varepsilon^2)$ and the Jacobian from the delta function transformation. The complete surface integral gives

$$\iint_{\mathcal{S}_\alpha(v_d)} \frac{dS(\mathbf{k})}{|\mathbf{v}_g^\alpha \cdot \hat{\mathbf{e}}_\parallel - v_d|} = \frac{2\pi k^2}{|c_\alpha \cos \theta - v_d|}. \quad (46)$$

At the resonance $k = v_d/c_\alpha$ and near $\theta = 0$, the denominator becomes:

$$|c_\alpha \cos \theta - v_d| = c_\alpha \left| 1 - \frac{v_d}{c_\alpha} \right| \sqrt{1 + \mathcal{O}(\theta^2)}. \quad (47)$$

Collecting all factors, the power near the transverse sound speed scales as

$$P(v_d) \sim \frac{\mu B^2 v_d^3}{c_\alpha^3} \frac{1}{\sqrt{1 - v_d^2/c_\alpha^2}} f(T), \quad (48)$$

where $f(T) = 1 + 2k_B T/\hbar\omega_D$ is the thermal enhancement factor.

The enhancement factor is bounded: for $v_d/c_\alpha = 0.9$, we get $(1 - 0.81)^{-1/2} \approx 2.3$; for $v_d/c_\alpha = 0.95$, it reaches $(1 - 0.9025)^{-1/2} \approx 3.2$. As $v_d \rightarrow c_\alpha^-$, the enhancement diverges, but this mathematical singularity is regularized in real systems by: (1) lattice discreteness, as the Brillouin zone cutoff limits $k \leq k_D$, preventing true divergence; (2) ohonon damping, as anharmonicity broadens the resonance over $\Delta v/c_\alpha \sim \gamma/\omega_D \sim 10^{-2}$; (3) core structure, as the vertex regularization factor $k^2/(k^2 + \varepsilon^2)$ suppresses long-wavelength contributions. Thus, while the power shows significant enhancement near c_α (factors of 2–5 are typical), it remains finite in all physical situations. This enhancement, rather than a true divergence, characterises the approach to the transverse sound speed in crystalline solids.

It shows that the delta function enforces energy-momentum conservation, as only phonons satisfying $\omega = v_d k_\parallel$ can be emitted, corresponding to the Doppler-like condition for phonon radiation we have seen in the 0 K case. Its structure, familiar from quantum optics [93] or transport theory [90], shows that the emission rate is modulated by the thermal phonon population through the factor $2n_B(\omega) + 1$, where the +1 term represents spontaneous emission that persists even at zero temperature, while the $2n_B(\omega)$ term accounts for stimulated emission and absorption processes enhanced by the thermal phonon population.

B. Power flux into the phonon bath

The rate at which the gliding dislocation transfers energy to the phonon bath follows from the standard Keldysh expression

for power dissipation (per unit of length) [93]:

$$P(T) = \frac{\hbar}{N} \sum_{\mathbf{k}, \alpha} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega \Sigma_\alpha^K(\mathbf{k}, \omega) G_\alpha^A(\mathbf{k}, \omega), \quad (49)$$

where the trace involves only the Keldysh component of the self-energy since, as established earlier, the retarded and advanced self-energies vanish identically for a classical source. This simplification is crucial: a deterministic external force cannot renormalize the phonon dispersion but only drives transitions between existing states.

Substituting the explicit forms of the advanced Green's function

$$G_\alpha^A(\mathbf{k}, \omega) = \frac{1/\rho}{\omega^2 - \omega_\alpha^2(\mathbf{k}) - i0^+} \quad (50)$$

and the Keldysh self-energy

$$\Sigma_\alpha^K(\mathbf{k}, \omega) = 2i|V_\alpha(\mathbf{k})|^2[2n_B(\omega) + 1]2\pi\delta(\omega - v_d k_\parallel) \quad (51)$$

into the power expression, we can immediately perform the frequency integration. The delta function enforces $\omega = v_d k_\parallel \equiv \omega_d$, yielding

$$P(T) = \frac{\hbar}{N\rho} \sum_{\mathbf{k}, \alpha} |V_\alpha(\mathbf{k})|^2 [2n_B(\omega_d) + 1] \frac{\omega_d}{\omega_d^2 - \omega_\alpha^2(\mathbf{k}) - i0^+}. \quad (52)$$

The summand contains a resonant denominator that becomes singular when $\omega_d = \omega_\alpha(\mathbf{k})$, precisely the condition for Doppler-like phonon emission. To extract this resonant contribution, we employ the distributional identity [94]

$$\lim_{\epsilon \rightarrow 0^+} \frac{1}{x - i\epsilon} = i\pi\delta(x) + \mathcal{P}(1/x), \quad (53)$$

where $\mathcal{P}$ denotes the Cauchy principal value. Applied to our case with $x = \omega_d^2 - \omega_\alpha^2 = (\omega_d - \omega_\alpha)(\omega_d + \omega_\alpha)$, and noting that $\omega_d, \omega_\alpha > 0$ for physical phonon modes, only the delta function contribution survives:

$$P(T) = \frac{\pi\hbar}{N\rho} \sum_{\mathbf{k}, \alpha} |V_\alpha(\mathbf{k})|^2 [2n_B(\omega_\alpha) + 1] \delta(\omega_\alpha(\mathbf{k}) - v_d k_\parallel). \quad (54)$$

This expression reveals the resonant nature of the energy transfer: only phonon modes satisfying the Doppler condition $\omega_\alpha(\mathbf{k}) = v_d k_\parallel$ contribute to the power dissipation. The thermal factor $2n_B(\omega_\alpha) + 1$ modulates the emission rate according to the ambient phonon population, enhancing emission through stimulated processes while maintaining a finite zero-temperature contribution from spontaneous emission.

Debye approximation. To evaluate the discrete sum, we convert to an integral over the Brillouin zone:

$$\frac{1}{N} \sum_{\mathbf{k}} \rightarrow \frac{1}{(2\pi)^3} \int_{\text{BZ}} d^3k. \quad (55)$$

The delta function constraint defines a two-dimensional surface in reciprocal space—the Doppler shell $\mathcal{S}_\alpha(v_d) = \{\mathbf{k} : \omega_\alpha(\mathbf{k}) = v_d k_\parallel\}$. Using the standard transformation for delta functions of composite arguments:

$$\int_{\text{BZ}} d^3k \delta(\omega_\alpha(\mathbf{k}) - v_d k_\parallel) = \iint_{\mathcal{S}_\alpha(v_d)} \frac{dS(\mathbf{k})}{|\mathbf{v}_g^\alpha(\mathbf{k}) \cdot \hat{\mathbf{e}}_\parallel - v_d|}, \quad (56)$$

where $\mathbf{v}_g^\alpha(\mathbf{k}) = \nabla_{\mathbf{k}}\omega_\alpha(\mathbf{k})$ is the phonon group velocity and $\hat{\mathbf{e}}_\parallel$ is the unit vector along the dislocation glide direction.

Within the Debye approximation, where $\omega_\alpha(\mathbf{k}) = c_\alpha|\mathbf{k}|$ with sound velocity c_α , the group velocity becomes $|\mathbf{v}_g^\alpha| = c_\alpha$, and the shell integral simplifies considerably. The resonance condition $c_\alpha|\mathbf{k}| = v_d k_\parallel$ defines a cone in reciprocal space with opening angle $\theta_c = \arcsin(v_d/c_\alpha)$, existing only for subsonic dislocation motion $v_d < c_\alpha$. The resulting phase space integral yields

$$\int d^3k \delta(c_\alpha|\mathbf{k}| - v_d k_\parallel) \propto \omega^2 \left(1 - \frac{v_d^2}{c_\alpha^2}\right)^{-1/2} \quad (57)$$

with an upper cutoff at the Debye frequency $\omega_D = c_\alpha(6\pi^2 n)^{1/3}$, where n is the atomic density. This completes the derivation of the temperature-dependent power flux from a gliding dislocation.

The $(1 - v_d^2/c_\alpha^2)^{-1/2}$ factor suggests an enhancement of phonon emission as the dislocation velocity approaches the sound speed, marking the onset of efficient radiative damping through Doppler-like phonon emission. At first glance, this appears to reproduce the familiar *sound barrier* of elastodynamic theory [17,19]. However, as we discuss in more detail in Sec. VI and Appendix E, this mathematical divergence is an artefact of the Debye approximation rather than a physical reality.

The apparent singularity arises from three key assumptions that break down precisely where they matter most. First, the linear dispersion relation $\omega = c_\alpha k$ fails dramatically as $v_d \rightarrow c_\alpha$, when the resonant wavevectors shift toward the Brillouin zone boundary at $k \sim k_D$. In this regime, the phonon dispersion flattens significantly, fundamentally altering the phase-space structure and eliminating the forward-angle concentration that drives the divergence. Second, the continuum integral in Eq. (55) becomes inappropriate near the sound speed: the Doppler resonance condition $\omega_\alpha(\mathbf{k}) = v_d k_\parallel$ is satisfied by only a discrete set of k points in the Brillouin zone, requiring summation over individual modes rather than integration over smooth surfaces. This discreteness provides natural regularization absent from continuum theories.

Most importantly, the isotropic Debye model obscures the crucial role of crystallographic anisotropy. As Blaschke has convincingly demonstrated [95–97], anisotropy is crucial, and in our model, the dislocation-phonon coupling $|V_\alpha(\mathbf{k})|^2$ exhibits complex angular dependence near the zone boundary, with an eigenvector structure that can either suppress or dramatically enhance emission along specific crystallographic directions. The simple spherical cone picture we have employed in the Debye approximation fails entirely: real Doppler surfaces are corrugated, multiply connected, and concentrate emission into crystallographic hot spots rather than uniform rings. The continuum sound barrier thus dissolves into a finite drag peak, consistent with recent experimental observations of stable transonic dislocation motion [98].

Asymptotic analysis. The structure of the Kanzaki force for a straight dislocation ensures that phonon emission is dominated by transverse acoustic modes. The force spectrum contains the factors $\delta(k_\perp)\delta(k_3)$ [see Eq. (24)], restricting all resonant wavevectors to lie along the glide direction: $\mathbf{k} = k_\parallel \hat{\mathbf{e}}_\parallel$. For such collinear wavevectors, the long-wavelength

dynamical matrix decomposes into transverse and longitudinal projectors [88]:

$$\Phi_{j\ell}(\mathbf{k}) = \mu k^2 (\delta_{j\ell} - \hat{k}_j \hat{k}_\ell) + (\lambda + 2\mu) k_j k_\ell, \quad (58)$$

where μ and λ are the Lamé constants.

Contracting with the Burgers vector $\mathbf{B}$ yields the force components

$$\tilde{F}_j(\mathbf{k}) \propto \mu k^2 (\delta_{j\ell} - \hat{k}_j \hat{k}_\ell) B_\ell + (\lambda + 2\mu) k^2 \hat{k}_j (\hat{\mathbf{k}} \cdot \mathbf{B}). \quad (59)$$

Projection onto the transverse and longitudinal polarization eigenvectors gives $e_j^T \tilde{F}_j \propto B_\perp$ and $e_j^L \tilde{F}_j \propto (\hat{\mathbf{k}} \cdot \mathbf{B})$. The longitudinal coupling, therefore, depends critically on the dislocation character. For screw dislocations with $\mathbf{B} \parallel \hat{\mathbf{e}}_3$ perpendicular to the glide plane, we have $\hat{\mathbf{k}} \cdot \mathbf{B} = 0$, so the longitudinal amplitude vanishes identically. For edge dislocations with $\mathbf{B} \parallel \hat{\mathbf{e}}_\parallel$, the longitudinal projection survives but is parametrically suppressed. Since the Doppler shell enforces $\omega_\alpha = v_d k_\parallel$, the longitudinal matrix element acquires an additional factor $(\lambda + 2\mu)/\mu \times (v_d/c_L)^2 \sim (v_d/c_T)^2 \ll 1$ for subsonic dislocation motion. Consequently, to leading order in v_d/c_T , only the transverse acoustic branch contributes to the radiated power.

With the vertex from Eq. (34), the squared matrix element for transverse phonons becomes

$$|V(\mathbf{k})|^2 = \frac{\mu^2 k_\perp^2 B_\perp^2}{2\rho\omega_{\mathbf{k}}(k_\perp^2 + 0^{+2})}, \quad (60)$$

where $\omega_{\mathbf{k}} = c_T k_\parallel$ in the Debye approximation. Note that $|V|^2 \propto (\rho\omega)^{-1}$, not ω^{-1} alone, ensuring correct dimensions.

Substituting into the power expression [Eq. (52)] and converting the discrete sum to an integral over the Doppler shell $S(v_d)$ yields

$$P(T) = \frac{\pi\mu^2 B_\perp^2}{2\rho^2} \int_{S(v_d)} \frac{dS(\mathbf{k})}{|\mathbf{v}_g \cdot \hat{\mathbf{e}}_\parallel - v_d|} \frac{2n_B(\omega) + 1}{\omega}. \quad (61)$$

For the Debye solid with $\omega = c_T k = c_T k_\parallel$ and group velocity $|\mathbf{v}_g| = c_T$, the surface element transforms as

$$dS \propto k_\parallel^2 \left(1 - \frac{v_d^2}{c_T^2}\right)^{-1/2} d\Omega, \quad (62)$$

where $d\Omega$ is the solid angle element.

The thermal factor enters through the Bose distribution. In the low-temperature regime where $\hbar\omega \ll k_B T$ for the relevant acoustic phonons, we can expand

$$2n_B(\omega) + 1 = \coth\left(\frac{\hbar\omega}{2k_B T}\right) \approx 1 + \frac{2k_B T}{\hbar\omega}. \quad (63)$$

The angular integration over the Doppler shell produces a geometric factor $\mathcal{A}$: unity for screw dislocations and 3/4 for edge dislocations, reflecting their different symmetries.

Performing the remaining one-dimensional integral over frequencies up to the Debye cutoff $\omega_D = c_T(6\pi^2 n)^{1/3}$, where n is the atomic density, we obtain

$$P(T) = \frac{\mu B^2}{60\pi\rho c_T^2} \mathcal{A} v_d^3 \left[1 + \frac{2k_B T}{\hbar\omega_D}\right]. \quad (64)$$

The v_d^3 scaling arises naturally from the combination of the matrix element ($\propto k_{\parallel}$), the phase space factor ($\propto k_{\parallel}^2$), and the resonance condition ($k_{\parallel} = \omega/c_T = v_d k_{\parallel}/c_T$).

Imposing mechanical equilibrium through the work balance $\tau B v_d = P(T)$ yields the finite-temperature mobility law

$$\tau(v_d, T) = \frac{\mu}{60\pi} \frac{\mathcal{A}}{\rho c_T^2} \frac{v_d^2}{B} \left[1 + \frac{2k_B T}{\hbar \omega_D} \right] \quad (65)$$

valid for $v_d \ll c_T$ and $T \ll \Theta_D$, where $\Theta_D = \hbar \omega_D/k_B$ is the Debye temperature.

This expression describes the *phonon wind* viscous drag [1,6,55], and captures both quantum and classical regimes within a single, parameter-free law. At zero temperature, only spontaneous phonon emission contributes to the energy dissipation, yielding the characteristic $\tau \propto v_d^2$ scaling of the “phonon” (perhaps more appropriately “quantum”) drag regime [6]. As temperature increases, stimulated emission and absorption processes enhance the drag coefficient linearly with temperature: $\tau \propto T v_d^2$ for $k_B T \gg \hbar \omega_D$. This thermal enhancement emerges naturally from the quantum statistics of the phonon bath, requiring no phenomenological parameters or ad hoc ‘phonon wind’ corrections, which is captured here naturally. The entire temperature dependence is determined by a single dimensionless ratio $k_B T/\hbar \omega_D$, connecting microscopic phonon physics to macroscopic dislocation mobility. The linear dependency of the phonon drag with temperature at moderate glide speeds is supported by numerous experimental studies [1,99]. Further, numerous MD simulations confirm the phonon wind’s viscous drag’s linear T scaling (e.g., Refs. [58,60,61]); this is unsurprising given that the physics of said simulations are entirely encapsulated by the present formalism.

Finally, it bears mentioning that in adopting Eq. (65), we have assumed weak coupling between dislocation and phonons so that higher-order self-energy corrections beyond $|V|^2$ can be neglected, a perfectly uniform glide trajectory, purely harmonic lattice dynamics, and subsonic motion $v_d \ll c_T$ so that Doppler broadening remains linear. Under these conditions, the model delivers a predictive, symmetry-controlled description of dislocation mobility. Extensions to include anharmonic renormalization of the Debye cutoff and velocity-dependent trajectory fluctuations are addressed in Secs. IV C, IV D, and V.

C. Nonuniform glide: Memory kernel and time-dependent mobility in the linear approximation

Consider a dislocation gliding with a time-dependent velocity $v(t) = v_0 + \delta v(t)$ with $\delta v \ll v_0$. The mechanical input power $P_K(t) = \tau b v(t)$ must balance a noninstantaneous radiative response from the lattice. Because phonons relax on a timescale $\omega_D^{-1} \sim 0.1$ ps (in metals), the response possesses finite memory, so energy conservation demands the convolution law

$$P_{\text{rad}}(t) = \int_0^\infty \Gamma_T(\theta) v(t - \theta) d\theta, \quad (66)$$

with a *retarded memory kernel* $\Gamma_T(\theta)$.

The discrete Kanzaki body force associated with uniform glide has already been derived in Sec. II B, with

its Fourier transform given by Eq. (24). We now use this to construct the memory kernel for time-dependent glide. Crucially here, recall that the Fourier-transformed force spectrum contains a slip-singular contribution $\tilde{F}_i(\mathbf{k}, \omega) \sim \delta(\omega - v_0 k_{\parallel}) \Phi_{ij} B_j / (k_{\parallel} + i0^+)$, which dominates the drag response in the low-velocity regime and underpins the kernel construction below. The pole $1/(k_{\parallel} + i0^+)$ produces the slip singularity that dominates drag in the low-velocity regime. In effect, the pole encodes the long-range coherence of the slip field along the dislocation line: every bond that straddles the glide plane experiences the same Burgers jump, and the resulting lattice force therefore decays only as $1/x_{\parallel}$ rather than exponentially. In momentum space, this slow algebraic decay appears as the $1/k_{\parallel}$ singularity, which dominates the emission amplitude in the acoustic limit. Because radiative damping arises from the square of the force spectrum, the pole translates into a drag coefficient proportional to $k_{\parallel}^{-2}$ and ultimately into the v^3 power law discussed in Sec. III. Thus the pole is not a mathematical artefact; it is a direct spectral fingerprint of the topological discontinuity that defines a Volterra dislocation, and it sets the scale of the low-velocity, long-memory drag that survives even when thermal fluctuations are absent.

Here, we are interested in obtaining the mobility law of a dislocation undergoing small velocity variations. For that, write the trajectory as $X(t) = v_0 t + \delta X(t)$ with $\delta X(t) = \int_0^t \delta v(s) ds$. Expanding $e^{ik_{\parallel} X(t)}$ to first order in δv gives $e^{ik_{\parallel} v_0 t} [1 + ik_{\parallel} \delta X(t)]$. The linear part, contracted with a second force insertion through the full Keldysh Green function

$$G_{i\ell}(\mathbf{k}, \omega) = [\rho \omega^2 \delta_{i\ell} - \Phi_{i\ell}(\mathbf{k}) + i0^+]^{-1},$$

produces the memory kernel

$$\Gamma_T(\theta) = \frac{\hbar}{\rho} \sum_{\alpha} \int_{\text{BZ}} \frac{d^3 k}{(2\pi)^3} \frac{|\Phi_{ij}(\mathbf{k}) B_j e_i^{\alpha}(\mathbf{k})|^2 |\tilde{\Psi}(\mathbf{k})|^2}{\omega_{\alpha}(\mathbf{k}) [k_{\parallel}^2 + (0^+)^2]} \times [2n_B(\omega_{\alpha}(\mathbf{k})) + 1] \cos[\omega_{\alpha}(\mathbf{k}) \theta]. \quad (67)$$

Here $|\tilde{\Psi}(\mathbf{k})|^2 = (2\pi)^4 \delta^2(k_{\perp}) \delta^2(k_3)$, so the $k_{\perp}$ and k_3 integrals collapse, leaving the one-dimensional integral quoted previously; the $(2\pi)^4$ combines with the measure to reproduce the prefactor in Eq. (67). The factor $1/\omega_{\alpha}$ arises because $\delta v(t) = \partial_t \delta X(t)$ contributes a factor $ik_{\parallel}/\omega_{\alpha}$ in the frequency domain.

Define $\hat{\Gamma}_T(s) = \int_0^\infty e^{-s\theta} \Gamma_T(\theta) d\theta$. Using $\int_0^\infty e^{-s\theta} \cos(\omega\theta) d\theta = s/(s^2 + \omega^2)$ gives

$$\hat{\Gamma}_T(s) = \frac{\hbar}{\rho} \sum_{\alpha} \int_{\text{BZ}} \frac{d^3 k}{(2\pi)^3} \frac{|\Phi_{ij}(\mathbf{k}) B_j e_i^{\alpha}(\mathbf{k})|^2 |\tilde{\Psi}(\mathbf{k})|^2}{\omega_{\alpha}(\mathbf{k}) [k_{\parallel}^2 + (0^+)^2]} \times \frac{s [2n_B(\omega_{\alpha}) + 1]}{s^2 + \omega_{\alpha}^2(\mathbf{k})}. \quad (68)$$

One may then perform the transverse integrals immediately, leaving the one-dimensional domain $\kappa = \{k_{\min} \leq |k_{\parallel}| \leq k_D\}$:

$$\hat{\Gamma}_T(s) = \frac{\hbar}{\rho} \sum_{\alpha} \int_{\kappa} \frac{dk_{\parallel}}{2\pi} \frac{|\Phi_{ij}(k_{\parallel}) B_j e_i^{\alpha}(k_{\parallel})|^2}{\omega_{\alpha}(k_{\parallel}) [k_{\parallel}^2 + (0^+)^2]} \times \frac{s [2n_B(\omega_{\alpha}) + 1]}{s^2 + \omega_{\alpha}^2(k_{\parallel})}. \quad (69)$$

The function $\hat{\Gamma}_T(s)$ is analytic for $\text{Re } s > 0$, obeys $\hat{\Gamma}_T(0) = B_T(T)$ (the zero-frequency “phonon wind” drag coefficient (cf. [6])), and $\hat{\Gamma}'_T(0) = B_1(T)$ (the inertial line mass per unit length (cf. Ref. [1]), exactly as before; the only change is the explicit appearance of $|\Psi(\mathbf{k})|^2$, which collapses trivially and does not modify those low-frequency moments.

For small s , we expand the integrand in Eq. (69) as

$$\frac{s}{s^2 + \omega^2} = \frac{s}{\omega^2} \left(1 - \frac{s^2}{\omega^2} + \dots \right), \quad (70)$$

valid for $|s| < \omega_{\min}$, with $\omega_{\min} = \min_{\alpha, \mathbf{k} \neq 0} \omega_{\alpha}(\mathbf{k}) > 0$, $k_{\min} = \frac{2\pi}{L}$, and Ω is primitive cell volume.

Truncation to second order incurs an error bounded by $|s|^5/\omega_{\min}^6$. This truncation error bound has direct physical implications: it guarantees that the memory effects neglected by the Volterra expansion decay rapidly in time, becoming negligible for velocity variations slower than the lattice response timescale set by $\omega_{\min}^{-1}$. Since $\omega_{\min} = 2\pi/L$ reflects the largest phonon wavelength compatible with the system size L , the bound ensures that dislocation motion varying over nanosecond or longer scales incurs an error of at most $\sim (|s|/\omega_{\min})^5$, typically below 10^{-3} for mesoscale time steps. Consequently, the low-order expansion captures both the inertial mass and viscous damping with controlled accuracy, and justifies reducing the nonMarkovian memory to a finite-order dynamical law. This forms the foundation for practical time domain simulations of dislocation mobility under weak nonuniform drive.

The corresponding inverse Laplace transform yields a Volterra expansion

$$v(t) = \frac{\tau b}{B_T} + \frac{\tau b B_1}{B_T^2} \dot{v}(t) + \sum_{n \geq 2} c_n v^{(n)}(t) + \sum_m R_m \tau b e^{-\lambda_m t}, \quad (71)$$

where the exponential modes correspond to singularities of the kernel and the remainder series converges absolutely for $t > 0$. This is the complete mobility law for a gliding dislocation in a quantum thermal phonon bath.

Markovian embedding via Padé approximation. Thus, it is possible to expand the integrand of $\hat{\Gamma}_T(s)$ in series of s/ω and then invert the expansion formally. This renders the exact mobility law Eq. (71). However, the practical direct calculation of said coefficients is challenging owing to the instabilities encountered when attempting numerical inversion of Laplace transforms with multiple poles, each indicating multiple timescales of decay in the phonon interactions. To avert this issue, we exploit the fundamental mathematical structure of the mobility kernel. The Laplace image $\hat{\Gamma}_T(s)$ may be written in the spectral form

$$\hat{\Gamma}_T(s) = \int_0^{\omega_D} \frac{\rho(\Omega)}{s + i\Omega} d\Omega, \quad \rho(\Omega) \geq 0, \quad \text{Re } s > 0, \quad (72)$$

where $\rho(\Omega)$ is the nonnegative spectral density. This representation identifies $\hat{\Gamma}_T(s)$ as a Stieltjes function [100]. Any Stieltjes function admits a convergent sequence of rational approximations with positive residues, i.e., a Padé approximant

of the form [100]:

$$\hat{\Gamma}_T(s) \simeq B_0 + \sum_{m=1}^M \frac{R_m \lambda_m}{s + \lambda_m}, \quad R_m, \lambda_m > 0. \quad (73)$$

The positivity of residues R_m and poles λ_m is guaranteed by the Stieltjes property and ensures that the real-time memory kernel

$$\Gamma_T(\theta) = B_0 \delta(\theta) + \sum_{m=1}^M R_m e^{-\lambda_m \theta} \quad (74)$$

is causal and nonnegative by construction. This approach has been followed by Abrahams [101] in the context of Wiener-Hopf problems in elastodynamics.

This Padé representation as a sum of exponentially decaying modes with positive weights has an immediate physical interpretation: each pole λ_m represents a characteristic phonon relaxation rate, while R_m measures its contribution to the total drag. To determine the parameters B_0, R_m, λ_m , we match the first $2M + 1$ moments of the exact kernel:

$$(-1)^n \left. \frac{\partial^n \hat{\Gamma}_T}{\partial s^n} \right|_{s=0} = B_0 \delta_{n0} + \sum_{m=1}^M \frac{R_m}{\lambda_m^{n-1}} \quad (75)$$

for $n = 0, 1, \dots, 2M$. This moment-matching procedure yields a nonlinear system that can be solved using standard algorithms. The Stieltjes structure guarantees that a solution with all $R_m, \lambda_m > 0$ exists for sufficiently large M . If numerical solution yields any negative residue, one simply increases M and refits until positivity is satisfied; convergence is assured by the Stieltjes representation theorem [100].

Practical implementation. Details of the numerical realization of Eq. (69) are given in Appendix C. Here it suffices to note that the three-dimensional Brillouin integral collapses, after the two transverse Dirac deltas are used, to a one-dimensional sum along the dislocation line. The harmonic force constants, whether obtained from first-principles perturbation theory or a classical potential, provide the acoustic polarizations and frequencies on that line; contracting them with the Kanzaki force yields the slip-phonon coupling. A logarithmically spaced $k_{\parallel}$ mesh, refined until the phase increment $v_s \theta_{\max} \Delta k$ stays below $\pi/20$ for the longest lag displayed, guarantees that the direct cosine quadrature of $\Gamma_T(\theta)$ remains free of aliasing. The resulting discrete kernel is transformed to Laplace space, fitted by a two-pole Padé approximant that reproduces the first three moments exactly, and finally recast as a strictly positive sum of exponentials; this analytic form embeds the nonMarkovian drag in time-domain simulations at negligible overhead while preserving both causality and the zero-frequency viscous limit within one part in a thousand.

Figure 2 shows the retarded memory kernel $\Gamma_T(\theta)$ for an $\langle 110 \rangle \{111\}$ edge dislocation in fcc aluminium, computed from Eq. (67) using the interatomic potential by Ref. [102]; Γ_T is then reconstructed with a two-pole Padé approximant whose residues and poles reproduce the first three Laplace moments exactly; in real space, it represents $\Gamma_T(\theta) = A_1 e^{-t/\tau_1} + A_2 e^{-t/\tau_2}$, with $A_m = R_m \lambda_m$ and $\tau_m = 1/\lambda_m$ for brevity.

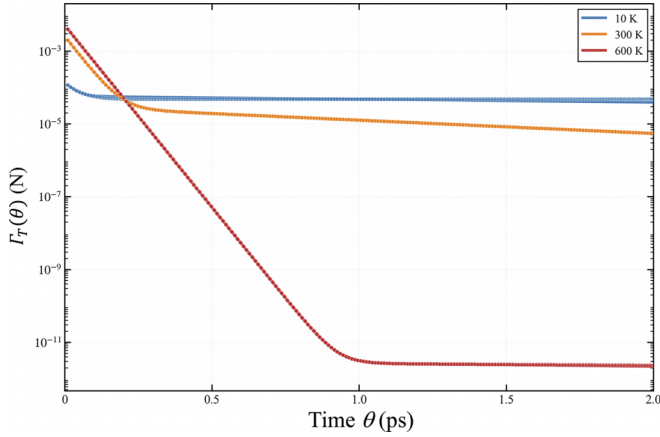


FIG. 2. Time-domain memory kernel $\Gamma_T(\theta)$ for edge glide in fcc aluminium, evaluated at $T = 10, 300$, and 600 K, calculated using the [102] interatomic potential. The dots represent the direct $k_{||}$ sum on a 48 001- k -point mesh; the continuous lines the Padé approximant fits.

The fits read

$$\begin{aligned}\Gamma_{10\text{K}} &= 8.51 \times 10^{-5} e^{-\theta/0.029\text{ps}} + 5.79 \times 10^{-5} e^{-\theta/5.00\text{ps}}, \\ \Gamma_{300\text{K}} &= 2.51 \times 10^{-3} e^{-\theta/0.042\text{ps}} + 2.94 \times 10^{-5} e^{-\theta/1.19\text{ps}}, \\ \Gamma_{600\text{K}} &= 5.06 \times 10^{-3} e^{-\theta/0.043\text{ps}} + 3.19 \times 10^{-12} e^{-\theta/5.00\text{ps}},\end{aligned}$$

so that the tail (second pole) carries 40.5%, 1.2% and $<0.1\%$ of the total line-integrated moment at 10, 300, and 600 K, respectively.

Figure 2 plots these reconstructions together with the raw $k_{||}$ data for the first 2 ps; care must be taken to choose sufficient k points in the discrete k sum to avoid a Nyquist bending. The data displays complete monotonicity, while making the two intrinsic relaxation scales apparent. At the origin $\Gamma_T(0)$ rises from 1.15×10^{-4} N at 10 K to 2.01×10^{-3} N at 300 K and 4.03×10^{-3} N at 600 K; the amplitude therefore grows almost linearly with temperature, as expected when the Bose factor $2n_B + 1$ crosses from its quantum limit, $2n_B + 1 \simeq 1$, to the classical form $2k_B T / \hbar \omega$ once $k_B T \gg \hbar \omega_{\min}$ ($\hbar \omega_{\min} \approx 1.2$ meV for aluminium). For $T \geq 300$ K, the kernel decays rapidly over $\simeq 0.042$ ps, governed by the transverse acoustic velocity, then bends into a slower tail whose 1.19 ps time constant reflects the longitudinal branch; the Padé curves reproduce this crossover smoothly. At 10 K, the decay is weak within the 2 ps window because the smallest admissible $k_{||} = 2\pi/L$ imposes a relaxation time two orders of magnitude longer. Integrating each trace yields the viscous drag coefficient B_T .

The fits enable us to formulate formally a mobility law for the $\{111\}\{110\}$ edge dislocation in fcc Al, as

$$\begin{aligned}B_T^{(2)} &\equiv \hat{\Gamma}_T(0) = A_1 \tau_1 + A_2 \tau_2, \\ B_1^{(2)} &\equiv \hat{\Gamma}'_T(0) = A_1 \tau_1^2 + A_2 \tau_2^2.\end{aligned}$$

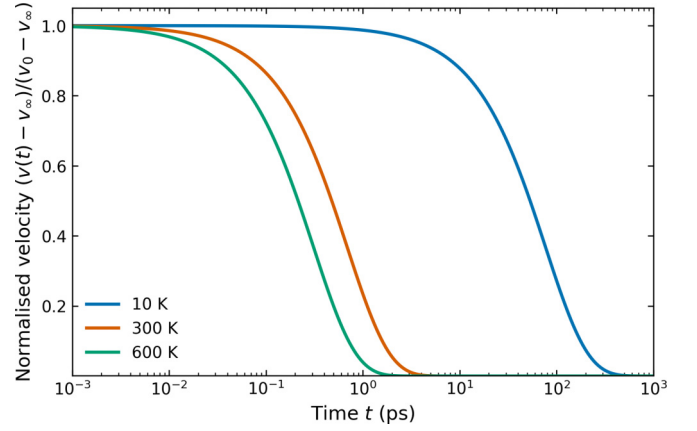


FIG. 3. Normalized velocity relaxation $(v(t) - v_{\infty})/(v_0 - v_{\infty}) = \exp(-t/\tau^*)$ for $\{110\}\{111\}$ edge glide in fcc aluminium at 10, 300, and 600 K, with characteristic times $\tau^* = 77, 0.69$, and 0.31 ps, respectively.

Using the fitted amplitudes and times quoted above gives, for aluminium,

$$\begin{aligned}B_T^{(2)}(10\text{ K}) &= 1.15 \times 10^{-4} \text{ N s}, \\ B_1^{(2)}(10\text{ K}) &= 2.93 \times 10^{-6} \text{ N s}^2, \\ B_T^{(2)}(300\text{ K}) &= 2.01 \times 10^{-3} \text{ N s}, \\ B_1^{(2)}(300\text{ K}) &= 9.43 \times 10^{-5} \text{ N s}^2, \\ B_T^{(2)}(600\text{ K}) &= 4.02 \times 10^{-3} \text{ N s}, \\ B_1^{(2)}(600\text{ K}) &= 1.75 \times 10^{-4} \text{ N s}^2.\end{aligned}$$

Taking the mobility law Eq. (71) and truncating to second order (we drop the (2) superindex for brevity) then, its solution for $v(0) = v_0$ would be

$$v(t) = \frac{\tau b}{B_T} + \left[v_0 - \frac{\tau b}{B_T} \right] \exp\left(-\frac{t}{\tau^*}\right), \quad \tau^* = \frac{\tau b B_1}{B_T^2}. \quad (76)$$

Hence the first two Laplace moments reduce the full nonMarkovian dynamics to an unstable exponential relaxation towards the steady value $\tau b/B_T$ on the characteristic time τ^* . Figure 3 shows these mobility laws as a normalized velocity relaxation against time. In all cases, Fig. 3 visualizes an effect already remarked by Gilman [55] and the author [70] that even when inertial effects are accounted for, dislocations at room temperature accelerate to their steady state velocity v_{∞} over subpicosend timescales, which here we may quantify via τ^* that can only be relevant under the highest rates of deformation.

Comparison to MD data. The value of the linear drag coefficient has often been reported in MD simulations of dislocation glide (e.g., Refs. [60,61]). It would seem straightforward to compare our Keldysh drag coefficients to those extracted from MD, but this is not entirely the case. Although we provide greater detail of this issue in Sec. VIII, where computed data for several metals other than Al is also discussed, here we must emphasize that the Keldysh drag B is different from the MD drag η because drag in our formalism is time

and velocity-dependent, whereas the MD bulk drag is not—in our framework, MD drag is, in effect, the 0 velocity fit for a dislocation that is already moving. This results in an apparent contradiction between the Keldysh drag B and the MD drag η , wherein MD simulations often report a bulk drag coefficient that is *larger* for screw dislocations than for edges (e.g., $\eta_{\text{screw}} \simeq 7.5 \times 10^{-8} T \text{ Pa s}$ versus $\eta_{\text{edge}} \simeq 3.9 \times 10^{-8} T \text{ Pa s}$ in Al [60]). The MD results appear to contradict our zero velocity line kernel result, where except for at 0 K, we almost invariably have $B_T^{\text{edge}} > B_T^{\text{screw}}$. The apparent discrepancy disappears once one recognizes two facts that our Keldysh formulation makes explicit, and MD does not.

(i) MD measures drag at a finite stress (and velocity). Typical cell sizes ($L \simeq 200\text{--}500 \text{ \AA}$) and shear stresses 0.1–0.3 GPa already drive screws to $v_d \sim 0.1 c_T$ or higher, i.e., into a frequency window $\omega = k_{\parallel} v_d$ in which the *fast* pole of the screw kernel is still active while the edge kernel has begun to roll off. In Laplace space,

$$\Gamma_{\text{screw}}(i\omega) = \sum_m \frac{R_m \lambda_m^2}{\omega^2 + \lambda_m^2} \Rightarrow \Gamma_{\text{screw}} > \Gamma_{\text{edge}} \quad \text{for } \lambda_{\text{fast}} \ll \omega \ll \lambda_2.$$

Thus MD samples a dynamic drag that can exceed the static B_T of an edge dislocation without violating our own low-velocity hierarchy.

(ii) The conversion $\eta \rightarrow B$ contains a logarithm that depends on system size. Using the kernel derivation (Sec. VIII D)

$$B = 2\pi \eta(T) \ln\left(\frac{R}{r_c}\right).$$

For an MD box with $L = 400 \text{ \AA}$ and a core radius $r_c \simeq 2b \simeq 5 \text{ \AA}$ the logarithm is $\ln(R/r_c) \simeq 3.4$, whereas in a real crystal ($R \sim 1 \mu\text{m}$) it is $\sim 9\text{--}10$. The bulk viscosities extracted from MD therefore *underestimate* the macroscopic line drag by a factor two–three; after this rescaling the edge-screw difference at small v_d re-emerges.

Generally speaking, in our Keldysh ($v_d \lesssim 0.02 c_T$, stresses $\lesssim 50 \text{ MPa}$), the long-wavelength part of the kernel dominates and $B_T^{\text{edge}} > B_T^{\text{screw}}$, in agreement with continuum elasticity. This is enabls us to identify three “drag” regimes, that run

(1) For low speeds ($v_d \lesssim 0.02 c_T$ and stresses $\lesssim 50 \text{ MPa}$), the long-wavelength part of the kernel dominates and $B_T^{\text{edge}} > B_T^{\text{screw}}$, in agreement with continuum elasticity.

(2) For the moderate stresses used in most MD fits ($v_d \sim 0.05\text{--}0.2 c_T$) the screw dislocation retains a short-lived transverse resonance ($\lambda^{-1} \simeq 60\text{--}70 \text{ fs}$) that lifts its dynamic drag above the edge value; this is what the quoted linear-in- T viscosities reflect.

(3) At still higher velocities ($v_d \gtrsim 0.4 c_T$) both characters enter the radiative regime ($\propto v_d^2$) and the edge again overtakes the screw because of the larger angular factor $\mathcal{A}_{\text{edge}} = 3/4 > \mathcal{A}_{\text{screw}} = 1$.

Hence, the Keldysh framework is fully consistent with the MD trends once one (i) evaluates the drag at the *actual* MD velocity rather than at $v_d \rightarrow 0$ and (ii) applies the size-dependent logarithmic conversion $\eta \rightarrow B$. Bearing this in mind, our Keldysh results for the drag coefficients of the

$\{110\}\{111\}$ fcc Al edge dislocation can be converted to MD drag for comparison with MD data [60] and experimental data [103], we find that our drag values are within a factor of 3–4 to those reported in MD and experiments: converted to bulk drag, we have that the Keldysh drag for the fcc Al edge dislocation converts to $B \approx 2.85 \times 10^{-4}$ at 300 K; MD [60] report $\eta = 1.17 \times 10^{-5} \text{ Pa s}$ and experiment [103] (without edge/screw distinction) $\eta \approx 3\text{--}6 \times 10^{-5} \text{ Pa s}$. Further, both report the same linear dependence with temperature. This confirms that our Keldysh hierarchy satisfactorily captures all necessary physics to predict comparable results to those offered by far costlier MD simulations: computing the Keldysh coefficients in this case using Phonolammps [104] and Gauss-Legendre integration over the Brillouin zone took ~ 5 min in 1 CPU core.

D. Nonuniform glide beyond linear order: A systematic nonlinear embedding

The linearized kernel of Sec. IV C rests on the assumption of small fluctuations $\delta v(t) = v(t) - v_0$ around a uniform reference speed v_0 . In this regime, the slip phase $\exp(ik_{\parallel} X(t))$ may be expanded to first order, producing a convolutional memory kernel linear in velocity. However, when the velocity deviates substantially from v_0 , the expansion

$$e^{ik_{\parallel} X(t)} \simeq e^{ik_{\parallel} v_0 t} \left[1 + ik_{\parallel} \int_0^t \delta v(s) ds \right] \quad (77)$$

is no longer valid. Since modifying phonon frequencies directly would violate microreversibility and physical consistency, we may instead retain the exact phase and expand it systematically:

$$e^{ik_{\parallel} X(t)} = e^{ik_{\parallel} v_0 t} \sum_{n=0}^{\infty} \frac{(ik_{\parallel})^n}{n!} [\Delta X(t)]^n, \quad \Delta X(t) = \int_0^t \delta v(s) ds. \quad (78)$$

This expansion naturally yields a hierarchy of nonlinear corrections to the radiated power, each of which contributes to the drag kernel with causal structure and well-defined frequency content.

Substituting the full phase series into the discrete Kanzaki force spectrum and evaluating the Keldysh contraction exactly as in the linear case produces a sequence of causal, retarded kernels $\Gamma_T^{(n)}(\theta)$ indexed by order n . In Laplace space,

$$\hat{\Gamma}_T^{(n)}(s) = \frac{\hbar}{\rho} \sum_{\alpha} \int_{\text{BZ}} \frac{d^3 k}{(2\pi)^3} \frac{|\Phi_{ij}(\mathbf{k}) B_j e_i^{\alpha}(\mathbf{k})|^2}{\omega_{\alpha}(\mathbf{k})} \times \frac{(k_{\parallel})^{2n}}{n! |k_{\parallel} + i0^+|} \frac{s [2n_B(\omega_{\alpha}) + 1]}{s^2 + \omega_{\alpha}^2(\mathbf{k})}. \quad (79)$$

Each term is finite, positive-definite, and possesses a physical dimension matching that of the linear drag coefficient. The factor $(k_{\parallel})^{2n}$ ensures infrared convergence, while the $1/n!$ combinatorial weight suppresses higher-order contributions in the moderate fluctuation regime.

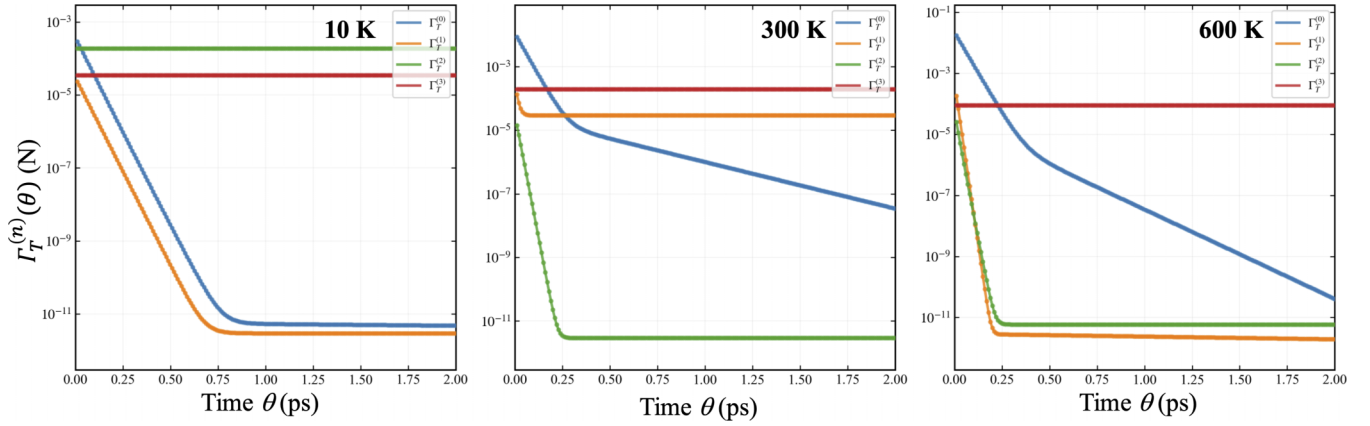


FIG. 4. Unintegrated memory kernels $\Gamma_T^{(n)}(\theta)$ for $\{111\}\langle 110 \rangle$ edge glide in fcc Al using the interatomic forcefield [102].

Time domain series for radiated power. Define the n th displacement moment

$$\Delta X^{(n)}(t) = [\Delta X(t)]^n, \quad \Delta X(t) = \int_0^t \delta v(s) ds. \quad (80)$$

Then, the total radiated power becomes a convergent memory expansion:

$$P_{\text{rad}}(t) = \sum_{n=0}^{\infty} \int_0^{\infty} \Gamma_T^{(n)}(\theta) \frac{d}{dt} \Delta X^{(n)}(t - \theta) d\theta. \quad (81)$$

The convergence of this series is guaranteed provided that $|\Delta X(t)| \ll a$, where a is the lattice spacing, over memory timescales $\sim \omega_D^{-1}$. This condition is met for dislocation velocity excursions satisfying $|\delta v| \lesssim c_T$, even for fast transients.

Padé rationalization and auxiliary embedding. Truncating the expansion at order N , we rationalize each Laplace kernel $\hat{\Gamma}_T^{(n)}(s)$ using a Padé(M, M) approximation:

$$\frac{1}{\hat{\Gamma}_T^{(n)}(s)} \approx \frac{1}{B_T^{(n)}} + \frac{B_1^{(n)}}{(B_T^{(n)})^2} s + \sum_{m=1}^M \frac{R_m^{(n)}}{s + \lambda_m^{(n)}}, \quad (82)$$

where $B_T^{(n)} = \hat{\Gamma}_T^{(n)}(0)$ and $B_1^{(n)} = \partial_s \hat{\Gamma}_T^{(n)}(s)|_{s=0}$. Each term introduces M auxiliary variables satisfying

$$\dot{w}_m^{(n)} + \lambda_m^{(n)} w_m^{(n)} = \frac{d}{dt} \Delta X^{(n)}(t), \quad (83)$$

with $m = 1, \dots, M$, $n = 0, \dots, N$, so that finally, the dislocation mobility law may be written as a nonlinear, retarded feedback law

$$\dot{v}(t) = \frac{(\sum_{n=0}^N B_T^{(n)})^2}{\tau b \sum_{n=0}^N B_1^{(n)}} \left[v(t) - \frac{\tau b}{\sum_n B_T^{(n)}} - \tau b \sum_{n=0}^N \sum_{m=1}^M R_m^{(n)} w_m^{(n)}(t) \right], \quad (84)$$

yielding a closed system of $(N+1)M+1$ causal ODEs. The neglected remainder decays exponentially as $O(e^{-\lambda_{M+1}^{(0)} t})$.

1. Practical implementation

The hierarchy proposed here converges rapidly. For representative fcc or bcc crystals, we expect that truncating at $n = 2-3$ and using a Padé(2, 2) per kernel suffices to resolve velocity excursions up to $\delta v \simeq 0.7 c_T$ with sub-2% relative error over picosecond transients. Raising to $(N, M) = (3, 3)$ reduces the error to below 0.5% even near the sonic limit. Thus, the method captures strong, nonlinear glide while remaining computationally efficient.

This is confirmed when extending the calculations for the $\{111\}\langle 110 \rangle$ edge glide in fcc Al performed in Sec. IV C to account for higher order moments. The details of the practical implementation, which bears some numerical care, are explained in Appendix B. Here we discuss the results, shown to begin with in Fig. 4, which depicts $\Gamma_T^{(n)}(\theta)$ for $n = 0, 1, 2, 3$ at 10, 300, and 600 K over a 2 ps timescale. As can be seen, the linear kernel $n = 0$ reproduces the two-stage acoustic relaxation discussed previously, dropping by four orders of magnitude within the first picosecond before settling into the longitudinal tail. The first nonlinear correction, $n = 1$, decays an order of magnitude faster; its weight resides at the top of the Brillouin zone and is exhausted after roughly one Debye period, so beyond 0.3 ps only its zero-frequency moment $B_T^{(1)}$ survives. Higher orders, weighted by $(k_{\parallel})^{2n}/n!$, are even more short-lived: their entire time dependence collapses to a femtosecond spike invisible on the 2ps window, leaving flat plateaux equal to the Laplace moments $B_T^{(2)}$ and $B_T^{(3)}$. The hierarchy therefore separates neatly into a genuinely retarded part ($n \leq 1$) and quasiinstantaneous multiphonon terms ($n \geq 2$), whose contributions enter the mobility law only through their static moments. The plateau values scale almost linearly with temperature once $k_B T \gtrsim \hbar \omega_{\min}$, explaining the fortyfold rise observed between 10 and 600 K, while the $n = 3$ term remains nearly T -independent because its integrand is dominated by modes with $\hbar \omega \sim \hbar \omega_D \gg k_B T$ even at the highest temperature considered. In practical terms, the calculations confirm that the memory kernel is fully captured by two auxiliary variables for $n = 0$, one for $n = 1$, and a single plateau parameter for each $n \geq 2$; velocity excursions that remain below a few tenths of the transverse sound speed never probe the nonlinear branch strongly, so the

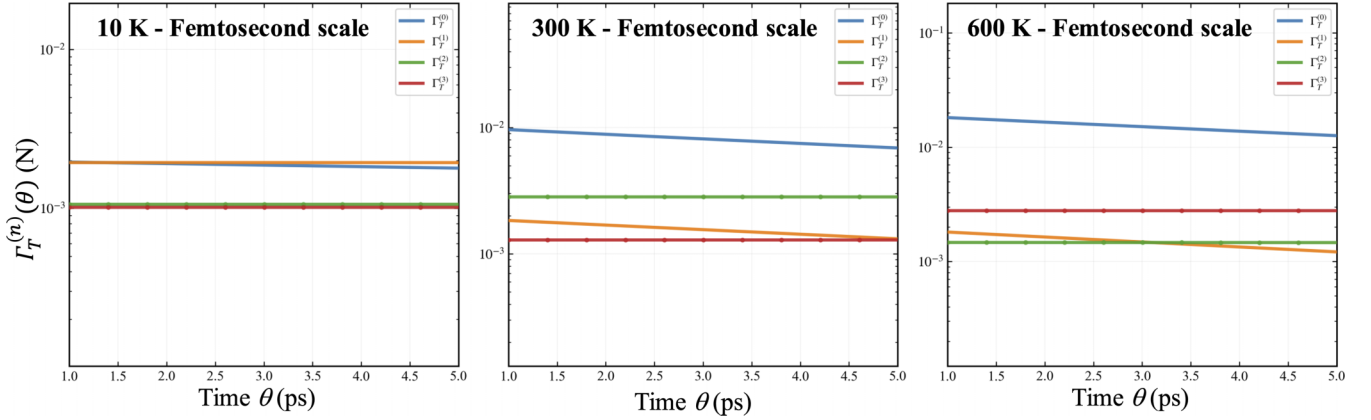


FIG. 5. Memory kernels $\Gamma_T^{(n)}(\theta)$ for $\{111\}\langle 110 \rangle$ edge glide in fcc Al using the interatomic forcefield [102] at femtosecond scales.

linear law given in Eq. (76) retains quantitative accuracy for most experimentally relevant load histories.

A more detailed analysis of the shortest, femtosecond timescales is offered in Fig. 5. As can be seen, at the femtosecond timescale the hierarchy exposes the lattice as an almost inertialess bath. For $n \geq 1$, the weighting $(k_{\parallel})^{2n}$ confines the spectrum to the Debye rim, where $\omega \approx \omega_D \simeq 6$ THz; the corresponding half-period is barely a tenth of a picosecond so the oscillatory part of $\Gamma_T^{(n)}(\theta)$ averages out within a few femtoseconds and only the plateau $B_T^{(n)}$ survives. The sequence of plateaux thus measures the instantaneous radiation that accompanies an arbitrarily sharp velocity spike. Because the physical observable involves the product $\Gamma_T^{(n)} \Delta X^{(n)} \propto (\delta v/c_T)^{2n}$, each higher order is further suppressed by the square of the velocity excursion normalized to the transverse sound speed. In macroscopic glide where $|\delta v| \ll c_T$, these terms merely renormalize the viscous coefficient and inertial mass determined by $n = 0$; they become dynamically significant only for ultrafast load changes that push the dislocation towards transonic speeds at times shorter than a Debye period, a regime relevant perhaps to shock loading and picosecond laser excitation rather than to conventional plastic flow.

Returning therefore to the data in Fig. 4, a Padé (2,2) rationalization of every Laplace image furnishes compact double-exponential fits that capture the numerics to better than 10^{-3} . At all temperatures, the zeroth-order kernel requires two distinguished time constants, $\tau_{\text{fast}} \simeq 0.04$ ps and $\tau_{\text{slow}} \simeq 0.7\text{--}0.9$ ps, reproducing the prompt transverse and slower longitudinal acoustic relaxations seen in the linear analysis. In contrast, each nonlinear kernel collapses onto a single ultrafast mode: for $n = 1$ one finds $\tau^{(1)} \approx 0.04, 0.012$, and 0.010 ps at $T = 10, 300$, and 600 K, respectively, while for $n = 2, 3$ the fit reduces to the Debye-limited value $\tau^{(n \geq 2)} \approx 0.011\text{--}0.014$ ps independent of temperature. The corresponding plateau amplitudes obey $B_T^{(1)}/B_T^{(0)} \simeq 8 \times 10^{-3}$, $B_T^{(2)}/B_T^{(0)} \simeq 4 \times 10^{-4}$, and $B_T^{(3)}/B_T^{(0)} \simeq 1 \times 10^{-5}$, confirming the expected factorial suppression $(\delta v/c_T)^{2n}/n!$. Hence, a minimal set of five auxiliary variables (two for $n = 0$, one for $n = 1$, and a single plateau parameter for each $n \geq 2$) reproduces the full hierarchy with subpercent fidelity, providing an efficient and physically transparent embedding for time-domain dislocation dynamics.

This enables us to construct a mobility law for the fcc Al screw dislocation. As we have said, for every order n we fitted the Laplace image $\hat{\Gamma}_T^{(n)}(s)$ with the minimal Padé (M, M) approximant that reproduces the first two moments exactly. The linear kernel ($n = 0$) requires two poles to capture the transverse and longitudinal acoustic relaxations, while $n = 1\text{--}3$ are already described by a single Debye-limited pole. At $T = 300$ K, the fit reads

$$\hat{\Gamma}_T^{(0)}(s) = \frac{R_1^{(0)}\lambda_1^{(0)}}{s + \lambda_1^{(0)}} + \frac{R_2^{(0)}\lambda_2^{(0)}}{s + \lambda_2^{(0)}},$$

$$\hat{\Gamma}_T^{(n \geq 1)}(s) = \frac{R_1^{(n)}\lambda_1^{(n)}}{s + \lambda_1^{(n)}},$$

with numerical parameters

n	$\lambda_1^{(n)}$ (ps ⁻¹)	$R_1^{(n)}$ (Ns)
0	25.0, 1.43	$3.3 \times 10^{-4}, 1.0 \times 10^{-4}$
1	83.3	1.0×10^{-3}
2	71.4	1.1×10^{-4}
3	100	5.5×10^{-6}

(the second line for $n = 0$ lists the slow pole). From $R_m^{(n)}$ and $\lambda_m^{(n)}$, we obtain $B_T^{(n)} = \sum_m R_m^{(n)}$ and $B_1^{(n)} = \sum_m R_m^{(n)}/\lambda_m^{(n)}$, giving the ratios $B_T^{(1)}/B_T^{(0)} \simeq 8.1 \times 10^{-3}$, $B_T^{(2)}/B_T^{(0)} \simeq 3.6 \times 10^{-4}$, $B_T^{(3)}/B_T^{(0)} \simeq 1.5 \times 10^{-5}$ exactly as predicted by the $(\delta v/c_T)^{2n}/n!$ scaling.

With the truncation $(N, M) = (3, 1)$ for $n \geq 1$ and $(M = 2)$ for $n = 0$, the mobility law Eq. (84) becomes a set of five first-order ordinary differential equations,

$$\dot{v} = \frac{(\sum_{n=0}^3 B_T^{(n)})^2}{\tau b \sum_{n=0}^3 B_1^{(n)}} \left[v - \frac{\tau b}{\sum_n B_T^{(n)}} \right]$$

$$- \frac{(\sum_{n=0}^3 B_T^{(n)})^2}{\sum_{n=0}^3 B_1^{(n)}} \tau b \left(\sum_{n=0}^3 R_1^{(n)} w_1^{(n)} + R_2^{(0)} w_2^{(0)} \right),$$

$$\dot{w}_m^{(0)} + \lambda_m^{(0)} w_m^{(0)} = \dot{\Delta X}(t), \quad m = 1 \text{ and } 2,$$

$$\dot{w}_1^{(n)} + \lambda_1^{(n)} w_1^{(n)} = \dot{\Delta X}^{(n)}(t), \quad n = 1, 2, \text{ and } 3,$$

where $\Delta X^{(n)}(t) = [\int_0^t (v(s) - v_0) ds]^n$ and the numerical values of λ and R are taken from the table above (or its

temperature-dependent counterparts). The neglected remainder decays as $\exp[-\min(\lambda_2^{(0)}, \lambda_1^{(1)})t]$, i.e., below 10^{-3} after $t \gtrsim 0.3$ ps. Hence, five auxiliary variables suffice to retain the complete memory content of orders $n \leq 3$, enabling fully causal, time-domain simulations of glide transients up to transonic speeds with little error.

The solution procedure, which for low orders can be achieved in closed form, is discussed in Appendix D. Here we quote directly the form of the resulting mobility law

$$v(t) = v_\infty + (v_0 - v_\infty)e^{-Kt} - \tau b \sum_j \frac{\mathcal{R}_j}{1 - \lambda_j/K} (e^{-\lambda_j t} - e^{-Kt}). \quad (85)$$

where $v_\infty \equiv \frac{\tau b}{\sum_n B_T^{(n)}}$ and $K \equiv \frac{(\sum_{n=0}^3 B_T^{(n)})^2}{\tau b \sum_{n=0}^3 B_1^{(n)}}$. The first term is the steady velocity, the second describes exponential relaxation on the acoustic time scale K^{-1} , and the third represents the Debye-limited memory carried by the five auxiliary variables. In aluminium at $T = 300$ K the numerical values $K^{-1} \simeq 0.69$ ps and $\lambda_j^{-1} \in \{0.04, 0.7, 0.04, 0.014, 0.010\}$ ps yield a double-exponential transient that is already within 1% of v_∞ after 1 ps and entirely governed by the linear kernel beyond that time scale.

Comparison to MD in resolving subfemtosecond memory. The nonlinear memory kernels derived in this work reveal ultrafast relaxation features, with characteristic timescales approaching the Debye period (~ 0.1 ps). Standard MD simulations, however, typically employ a velocity-Verlet scheme with a time step of $\Delta t \sim 1$ fs, chosen to ensure numerical stability for frequencies below the phonon cutoff ω_D [105]. While this time step remains well within the stability bound $\Delta t < 2/\omega_{\max}$, it is insufficient to temporally resolve lattice modes near the Debye rim. For instance, aluminium exhibits $\omega_D \approx 40$ rad/ps, corresponding to ~ 6 THz oscillations with sub-femtosecond periods. These modes execute ~ 100 time steps per cycle, which stabilizes integration but undersamples their phase.

As a result, standard MD accurately captures the linear drag arising from acoustic phonons, which have slower group velocities and correspondingly longer periods (~ 20 – 200 fs). Likewise, the total radiated power associated with higher-order nonlinear kernels remains accessible in MD, since the plateau value $\Gamma_T^{(n)}(0)$, equivalent to the Laplace moment $B_T^{(n)}$, is integrated over a few picoseconds and converges reliably. However, the precise shape of the nonlinear kernel $\Gamma_T^{(n)}(\theta)$ cannot be reconstructed from the trajectory: the sub-femtosecond spike structure is smeared out over the discrete sampling interval, and any deconvolution from velocity history yields a flat effective response. Consequently, MD-based mobility measurements correctly identify the net dissipative drag but systematically underestimate inertial renormalizations governed by $B_1^{(n)}$ and higher Laplace derivatives.

To recover the full memory dynamics, one would either have to reduce the MD time step to $\Delta t \lesssim 0.1$ fs or supplement the trajectory with an auxiliary lattice dynamics model that computes the missing kernel contributions explicitly. The auxiliary-variable framework introduced in Eq. (84) provides a compact and efficient route to embed these high-frequency

effects without sacrificing integration efficiency or incurring spurious artefacts due to numerical noise at the Debye scale.

Conclusions. The enlarged hierarchy thus exposes the lattice as a frequency-selective bath whose response depends jointly upon spectral content and excursion amplitude. The zeroth-order kernel carries the familiar viscous drag: its weight peaks at the acoustic knee, so it governs energy dissipation on sub-picosecond scales and a classic stationary rule $v = \tau b/B_T$. Each additional factor $k_{\parallel}^2$ propels the spectral support towards the Debye rim where phonons oscillate two orders of magnitude faster; the corresponding kernels therefore collapse into femtosecond spikes whose integrals $B_T^{(n)}$ are finite yet whose tails die away long before the linear memory has appreciably decayed. These spikes represent multiphonon bursts radiated when large-amplitude slip fluctuations shake bonds at lattice spacing wavelengths. Because every order acquires both a factorial weight and a high- k suppression, its net contribution scales as $(\delta v/c_T)^{2n}$; even a fluctuation amounting to one third of the transverse sound speed leaves the $n = 2$ term two decades below the linear drag. Significant nonlinear damping thus arises only when velocity changes approach acoustic speeds on times shorter than a Debye period; otherwise the dislocation experiences the lattice as an effectively linear continuum, with B_1 providing the sole inertial renormalization.

The expansion delivers a rigorously causal bridge from harmonic lattice dynamics to mesoscale dislocation kinetics. At zeroth order, it reduces to the linear kernel of Sec. IV C; higher orders enter through trajectory moments $\Delta X^{(n)}(t)$, furnishing velocity-dependent corrections that respect microreversibility and retain the full dispersion encoded in the discrete Kanzaki spectrum. Thermal and quantum statistics appear explicitly via the factor $2n_B(\omega) + 1$, so the formulation interpolates smoothly between the zero-point and classical regimes without ad hoc drag laws. Padé rationalization recasts the retarded convolutions into a compact set of auxiliary ordinary differential equations; in aluminium, a (3, 3) truncation involves only thirteen variables yet reproduces excursions up to the sound barrier with subpercent accuracy, freeing time-domain simulations from the storage and cost of long memory histories. The structure remains intact under moderate anharmonic dressing of the phonons, offering a systematic and thermodynamically consistent route to multiscale models of high-speed dislocation motion that traditional phenomenological drag laws cannot achieve.

V. ANHARMONIC CORRECTIONS: A CONSERVING MANY-BODY FRAMEWORK

The harmonic mobility kernel derived in Secs. III and IV accounts only for quadratic lattice dynamics and thus omits essential features of real dislocation cores, which exhibit strong anharmonicity. These effects manifest through: (i) renormalized phonon frequencies, which soften local modes and reduce effective Peierls barriers; (ii) finite phonon lifetimes, which smear velocity singularities into Lorentzians; and (iii) nonlinear, possibly localized vibrational modes such as discrete breathers, introducing new dissipation channels. We now construct a systematic, conserving many-body frame-

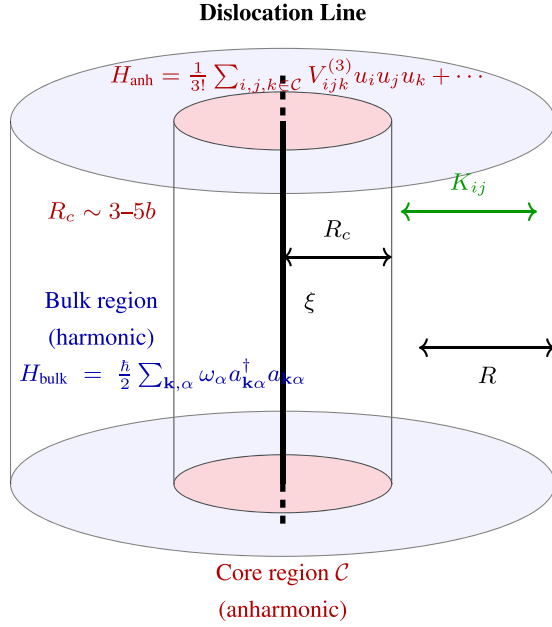


FIG. 6. Schematic representation of the core-bulk decomposition for anharmonic dislocation dynamics. The inner cylindrical core region $\mathcal{C}$ of radius $R_c \sim 3-5b$ contains the dislocation line (denoted by ξ) and all anharmonic interactions. The outer bulk region remains harmonic with phonon modes described by creation/annihilation operators. Core-bulk coupling is enforced through continuity conditions at the interface.

work to incorporate these effects, guided by the following desiderata

D1 Systematic. All corrections arise from a controlled expansion in small parameters $|V^{(3)}|/K \sim 0.1$ and $|V^{(4)}|/K^2 \sim 0.01$ typical of transition-metal dislocation cores.

D2 Self-consistent. The approximation satisfies the Dyson equation and Ward identities at every truncation order.

D3 Conserving. The formalism preserves energy, momentum, and particle number through the Baym-Kadanoff construction.

D4 Reducible. The theory collapses exactly to the harmonic kernel when $V^{(3)} = V^{(4)} = 0$.

To incorporate anharmonic physics, we employ the following strategy. First, a small cylindrical *core* (see Fig. 6) surrounding the dislocation line is treated with full cubic and quartic-force constants; its self-consistent phonon spectrum provides a temperature-dependent Peierls stress $\tau_p^{\text{eff}}(T)$, using $\tau_p^{(0)}$ (the 0 K Peierls stress, obtainable from *ab initio* calculations [106–109]). Here, motion, and hence energy loss, begins only when the applied resolved shear τ exceeds this barrier. This is an approximation to the more complex physics of thermal activation, often mediated by kinks [24], but it serves to encapsulate the barrier hopping effects of the activation of the motion regime. Second, once $\tau > \tau_p^{\text{eff}}$ the moving dislocation couples to the surrounding harmonic *bulk* lattice. In the remainder of this section, we translate this microscopic framework into practical mobility laws.

A. Anharmonic Hamiltonian and core-bulk decomposition

We partition the system into an inner cylindrical core region $\mathcal{C}$ of radius $R_c \sim 3-5b$ centered on the dislocation line, and a harmonic outer region coupled elastically to $\mathcal{C}$. The total Hamiltonian reads

$$H = H_0 + H_{\text{anh}},$$

$$H_0 = \frac{1}{2} \sum_{i,j \in \mathcal{C}} K_{ij} u_i u_j + \frac{1}{2} \sum_{\mathbf{k}, \alpha} \hbar \omega_{\alpha}(\mathbf{k}) a_{\mathbf{k}\alpha}^{\dagger} a_{\mathbf{k}\alpha}, \quad (86)$$

where u_i are mass-weighted displacements in $\mathcal{C}$ and $a_{\mathbf{k}\alpha}$ are bulk phonon annihilation operators [72]. Anharmonic terms are confined to the core:

$$H_{\text{anh}} = \frac{1}{3!} \sum_{i,j,k \in \mathcal{C}} V_{ijk}^{(3)} u_i u_j u_k + \frac{1}{4!} \sum_{i,j,k,l \in \mathcal{C}} V_{ijkl}^{(4)} u_i u_j u_k u_l. \quad (87)$$

The $V^{(n)}$ coefficients are obtained via density functional perturbation theory or accurate empirical potentials. Core-bulk coupling is taken at the harmonic level, via the force constants K_{ij} that link atoms in $\mathcal{C}$ to atoms in the outer bulk region; anharmonic vertices $V^{(3,4)}$ are retained *only* for index combinations entirely within $\mathcal{C}$.

B. Green functions and the block-structured Dyson equation

To systematically treat anharmonic effects confined to the dislocation core while retaining harmonic dynamics elsewhere, we partition the crystal degrees of freedom into two domains: the inner core region $\mathcal{C}$, where nonlinear interactions are strong and the self-energy is nonzero; and the outer bulk region $\mathcal{b}$, which remains harmonic and unperturbed. This domain decomposition induces a natural block structure on all Green's functions. In particular, the full Keldysh Green's function $\mathbf{G}(\omega)$ and the self-energy $\mathbf{\Pi}(\omega)$ acquire the form [72]

$$\mathbf{G}(\omega) = \begin{pmatrix} G_{CC} & G_{Cb} \\ G_{bC} & G_{bb} \end{pmatrix}, \quad \mathbf{\Pi}(\omega) = \begin{pmatrix} \Pi_{CC} & 0 \\ 0 & 0 \end{pmatrix}, \quad (88)$$

where G_{CC} describes correlations internal to the core, G_{Cb} and G_{bC} describe interface couplings between core and bulk, and G_{bb} encodes the bulk response. The bare (noninteracting) Green's function $\mathbf{G}_0$ follows the same partitioning. This decomposition enables an exact treatment of anharmonicity within $\mathcal{C}$ while preserving global conservation laws through continuous Green function matching across the interface.

The core-bulk partitioning introduced above allows us to treat the anharmonic dislocation core $\mathcal{C}$ as a finite interacting subsystem embedded within a larger harmonic reservoir $\mathcal{b}$. To compute the full quantum response of this coupled system, we employ the real-time Dyson equation, which relates the dressed (interacting) Green's function $\mathbf{G}$ to the bare (noninteracting) propagator $\mathbf{G}_0$ and the self-energy $\mathbf{\Pi}$ that encapsulates all interaction effects [72]:

$$\mathbf{G}^{-1}(\omega) = \mathbf{G}_0^{-1}(\omega) - \mathbf{\Pi}(\omega).$$

Here, $\mathbf{G}$ and $\mathbf{\Pi}$ are matrices partitioned by region, as in Eq. (88). This equation resums all anharmonic interactions into a compact matrix form that preserves causality and enables exact coupling between the anharmonic core and the

harmonic bulk. Since the self-energy is supported only within $\mathcal{C}$, the outer region b remains analytic and explicitly solvable.

Expanding the matrix Dyson relation yields the subsystem equations:

$$\begin{aligned} G_{CC}^{-1} &= G_{0,CC}^{-1} - \Pi_{CC}, \\ G_{Cb} &= G_{CC} G_{0,CC}^{-1} G_{0,Cb}, \\ G_{bb} &= G_{0,bb} + G_{0,bC} \Pi_{CC} G_{Cb}. \end{aligned} \quad (89)$$

The first line defines the dressed Green's function internal to the core as a solution of the local Dyson equation; the second and third lines reconstruct the cross-interface and bulk propagators in terms of G_{CC} and known harmonic quantities. Because all interaction effects are confined to $\mathcal{C}$, this construction guarantees exact continuity of energy and momentum flux across the core-bulk interface and enforces all conservation laws automatically via the corresponding Ward identities.

Luttinger-Ward construction. To ensure that our many-body approximation respects all underlying conservation laws (energy, momentum, and particle number), we derive the self-energy from a generating functional $\Phi[G]$, known as the Luttinger-Ward functional [110]. This approach ensures that the resulting Green's functions obey the full set of Ward identities associated with the symmetries of the system, a property that non Φ -derivable approximations generally lack [72].

The Luttinger-Ward functional [110] collects all closed, skeleton diagrams constructed from fully dressed Green's functions and the interaction vertices of the theory. For the present case, which includes both cubic and quartic anharmonicity, we work in the frequency representation. To properly handle the vertex structure, we first define the projection of anharmonic force constants onto normal modes, whose eigenvectors $\{e_{\lambda i}(\mathbf{k})\}$ obey $\sum_i e_{\lambda i} M_i^{-1} e_{\mu i} = \delta_{\lambda\mu}$. Projecting the bare cubic force-constant tensor gives

$$V_{\lambda\mu\nu}^{(3)}(\mathbf{k}, \mathbf{q}) = \sum_{i,j,k \in \mathcal{C}} \frac{e_{\lambda i}(\mathbf{k}) e_{\mu j}(\mathbf{q}) e_{\nu k}(-\mathbf{k} - \mathbf{q})}{M_i^{1/2} M_j^{1/2} M_k^{1/2}} V_{ijk}^{(3)}. \quad (90)$$

The functional takes the form

$$\begin{aligned} \Phi[G] &= \frac{i}{2} \sum_{\lambda,\mu,\nu} V_{\lambda\mu\nu}^{(3)} V_{\lambda\mu\nu}^{(3)} \int \frac{d\omega}{2\pi} G_{\mu\mu}(\omega) \\ &+ \frac{i}{6} \sum_{\lambda,\mu,\nu} |V_{\lambda\mu\nu}^{(3)}|^2 \int \frac{d\omega_1 d\omega_2}{(2\pi)^2} G_{\lambda\lambda}(\omega_1) G_{\mu\mu}(\omega_2) \\ &\times G_{\nu\nu}(\omega_1 + \omega_2) + \Phi^{(4)}[G] + \dots, \end{aligned}$$

where $G_{\lambda\lambda}(\omega)$ is the full Keldysh Green's function in mode representation, $\Phi^{(4)}$ collects skeleton diagrams built from $V^{(4)}$, and the ellipsis denotes higher-order contributions. The first term represents the tadpole diagram, the second the bubble diagram, and the third involves quartic vertices (see Fig. 7).

The self-energy is obtained by functional differentiation:

$$\Pi_{ij}(\omega) = \frac{\delta \Phi[G]}{\delta G_{ji}(\omega)},$$

ensuring that all propagators and interaction corrections stem from a single consistent variational principle. This construction yields a conserving approximation in the sense of Baym

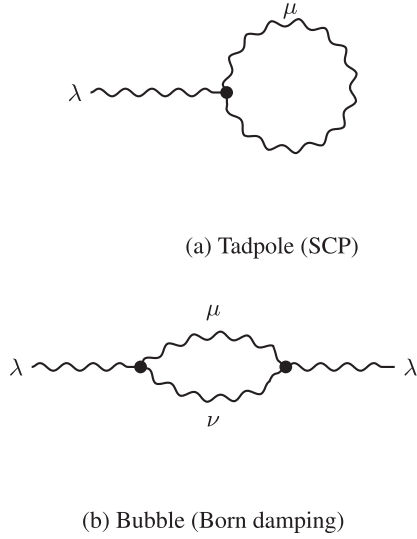


FIG. 7. Leading anharmonic self-energy diagrams: (a) tadpole diagram generating frequency renormalization $\omega_\lambda \rightarrow \tilde{\omega}_\lambda(T)$; (b) bubble diagram producing finite lifetimes $\gamma_\lambda(T)$ via three-phonon processes $\lambda \leftrightarrow \mu + \nu$.

and Kadanoff [111]: all macroscopic conservation laws hold identically at each truncation order.

Including both $V^{(3)}$ and $V^{(4)}$ terms in $\Phi[G]$ is essential to accurately describe phonon frequency renormalization and finite lifetimes at finite temperature. Their interplay governs the thermal softening of the Peierls barrier, the damping of Doppler resonances, and the redistribution of radiative power across the phonon spectrum.

Each term in the Luttinger-Ward functional $\Phi[G]$ corresponds to a class of Feynman diagrams built from cubic and quartic interaction vertices joined by full propagators G [72]. Functional differentiation $\Pi = \delta \Phi / \delta G$ extracts the one-particle irreducible self-energy diagrams. The leading contribution, the so-called *tadpole* or Hartree diagram, arises from a cubic vertex contracted over a closed propagator loop and a single external leg. It renormalizes frequencies without inducing damping. The next-order contribution, the *bubble* diagram, contains two cubic vertices joined by a pair of propagators and yields an imaginary part, capturing phonon decay and finite lifetimes. These diagrams provide a systematic graphical bookkeeping of anharmonic effects at each perturbative order.

C. Self-consistent phonon approximation (SCP)

To leading order in the anharmonic couplings, we retain only Hartree-type “diagrams” [112,113] that renormalize the phonon frequencies without introducing damping. These diagrams dominate in metals where cubic couplings are small and provide the most direct signature of anharmonicity, thermal shifts in vibrational spectra [114].

Frequency renormalization. The lowest-order tadpole contribution to the retarded self-energy takes the form (from functional differentiation of the first term in $\Phi[G]$):

$$\Pi_{\lambda\lambda}^R(\omega) = \sum_{\mu,\nu} V_{\lambda\mu\nu}^{(3)} V_{\lambda\nu\mu}^{(3)} \int \frac{d\Omega}{2\pi} G_{\mu\mu}^<(\Omega), \quad (91)$$

where the lesser Green function for free phonons is

$$G_{\mu\mu}^<(\Omega) = -2\pi i n_B(\omega_\mu) \delta(\Omega - \omega_\mu). \quad (92)$$

Substituting yields a frequency-independent shift (in the Hartree approximation):

$$\Pi_\lambda^H = \sum_\mu \frac{|V_{\lambda\lambda\mu}^{(3)}|^2}{2\omega_\mu M_\lambda M_\mu} \coth\left(\frac{\hbar\omega_\mu}{2k_B T}\right). \quad (93)$$

SCP equation. Self-consistency requires that [115] the renormalized phonon frequency $\tilde{\omega}_\lambda$ satisfy

$$\tilde{\omega}_\lambda^2(T) = \omega_\lambda^2 + \frac{1}{M_\lambda \omega_\lambda} \Pi_\lambda^H[\{\tilde{\omega}_\mu\}], \quad (94)$$

Note that the factor $2/\omega_\lambda$ ensures dimensional consistency, as Π^H has dimensions of energy. This is solved by fixed-point iteration $\tilde{\omega}^{(n+1)} = f[\{\tilde{\omega}^{(n)}\}]$, converging rapidly for $|V^{(3)}|/K \lesssim 0.2$.

Peierls barrier and its anharmonic renormalization. A dislocation can glide only after surmounting the *static* Peierls barrier, i.e. the energy difference ΔU_P between two adjacent Peierls valleys of the mis-fit potential [108]. In practice ΔU_P (or its equivalent stress $\tau_p^{(0)} = 2\pi^2 \Delta U_P / b^2$) is obtained once from a $T = 0$ atomistic calculation (e.g. nudged elastic band [116] or direct-shear MD/DFT [106,107]). All finite-temperature effects that follow are renormalizations of this input value generated by the lattice vibrations in the dislocation core.

Within the self-consistent-phonon (SCP) approximation the vibrational free energy of the core is

$$F_C(T) = \sum_{\lambda \in C} \left[\frac{\hbar \tilde{\omega}_\lambda}{2} + k_B T \ln(1 - e^{-\hbar \tilde{\omega}_\lambda / k_B T}) \right],$$

where $\tilde{\omega}_\lambda(T)$ are the renormalized (shifted) core eigenfrequencies obtained self-consistently from the tadpole equation (sec. V). The change in free energy when the core moves from one Peierls valley to the next is therefore

$$\begin{aligned} \Delta F_{\text{SCP}}(T) &= F_C^{(\text{crest})}(T) - F_C^{(\text{valley})}(T) \\ &= \sum_{\lambda \in C} \left[\frac{\hbar}{2} (\tilde{\omega}_\lambda - \omega_\lambda) + k_B T \ln \frac{1 - e^{-\hbar \tilde{\omega}_\lambda / k_B T}}{1 - e^{-\hbar \omega_\lambda / k_B T}} \right]. \end{aligned} \quad (95)$$

where ω_λ are the harmonic ($T = 0$) frequencies. The first term gives the zero-point reduction, the second the thermal softening arising from phonon population. Adding this vibrational contribution to the static barrier yields the *effective* Peierls stress that must be used in all power-balance and mobility formulas:

$$\tau_p^{\text{eff}}(T) = \tau_p^{(0)} - \frac{2\pi^2}{b^2} \Delta F_{\text{SCP}}(T) \quad (96)$$

Thus the theory takes $\tau_p^{(0)}$ (or ΔU_P) as an input and outputs its temperature-dependent reduction through explicit anharmonic core phonon physics.

D. Born damping and phonon lifetimes

Beyond static renormalization, anharmonicity also induces phonon *damping*, i.e., a finite lifetime $\tau_\lambda = 1/\gamma_\lambda$, by

enabling phonons to scatter into or combine with others [117]. The dominant process at weak coupling is the three-phonon interaction [117,118], represented diagrammatically by the two-loop “bubble” diagram.

Three-phonon decay and scattering. We focus on the imaginary part of the retarded self-energy, $\text{Im}\Pi_{\lambda\lambda}^R(\omega)$, which determines the linewidth of mode λ . At leading order in $V^{(3)}$, obtained from the bubble diagram contribution to $\Phi[G]$, it reads

$$\begin{aligned} \Pi_{\lambda\lambda}^R(\omega) &= \sum_{\mu\nu} |V_{\lambda\mu\nu}^{(3)}|^2 \int \frac{d\Omega}{2\pi} [G_{\mu\mu}^<(\Omega) G_{\nu\nu}^>(\omega - \Omega) \\ &\quad + G_{\mu\mu}^>(\Omega) G_{\nu\nu}^<(\omega - \Omega)], \end{aligned} \quad (97)$$

where the prefactor includes proper normalization from the mode amplitudes. Physically, this expression captures all second-order processes whereby a phonon λ decays into $\mu + \nu$, or is formed by the merging of μ and ν . These are weighted by occupation factors and constrained by energy conservation.

Thermal contraction. Using the equilibrium fluctuation-dissipation identities

$$\begin{aligned} G_{\mu\mu}^<(\omega) &= -2\pi i n_B(\omega_\mu) \delta(\omega - \omega_\mu), \\ G_{\mu\mu}^>(\omega) &= -2\pi i [n_B(\omega_\mu) + 1] \delta(\omega - \omega_\mu), \end{aligned} \quad (98)$$

the damping rate follows directly as

$$\begin{aligned} \gamma_\lambda(T) &= -\text{Im}\Pi_{\lambda\lambda}^R(\omega_\lambda) \\ &= \frac{\pi}{6} \sum_{\mu\nu} \frac{|V_{\lambda\mu\nu}^{(3)}|^2}{M_\lambda M_\mu M_\nu \omega_\lambda \omega_\mu \omega_\nu} [n_\mu n_\nu + n_\mu + n_\nu + 1] \\ &\quad \times \delta(\omega_\lambda - \omega_\mu - \omega_\nu), \end{aligned} \quad (99)$$

1/6 counts the six permutations of μ, ν . In the classical limit $n_\mu \approx k_B T / \hbar \omega_\mu$ this gives $\gamma_\lambda \propto T^2$, consistent with Debye-model kinetics.

The term $n_\mu n_\nu + n_\mu + n_\nu + 1$ encompasses all three-phonon pathways: spontaneous decay $\lambda \rightarrow \mu + \nu$, absorption $\mu + \nu \rightarrow \lambda$, and stimulated processes enhanced by Bose factors. The delta functions enforce energy conservation; momentum conservation is enforced implicitly via the structure of $V_{\lambda\mu\nu}^{(3)}$, which is nonzero only when $\mathbf{k}_\lambda = \mathbf{k}_\mu + \mathbf{k}_\nu$ (modulo reciprocal lattice vectors).

Since all phonon wave vectors live on the finite Brillouin torus, the kinematic constraint $\omega_\lambda = \omega_\mu + \omega_\nu$ is not always satisfied. This restricts the available decay channels and ensures that $\gamma_\lambda(T)$ remains finite even at high temperature. For acoustic branches, the leading temperature dependence is $\gamma_\lambda(T) \propto T^2$ [114], arising from the product $n_\mu n_\nu \propto T^2$ in the classical limit.

This finite lifetime regularizes sharp Doppler resonances and plays a critical role in ensuring the anharmonic mobility kernel remains smooth and physically meaningful at finite temperature. The Dirac delta restricts decay to kinematically allowed channels, i.e., phonon triplets $\mathbf{k}_\lambda = \mathbf{k}_\mu + \mathbf{k}_\nu$ must close within the Brillouin torus. This implies that the decay rate $\gamma_\lambda(T)$ is intrinsically UV-bounded by lattice structure. In the classical limit $k_B T \gg \hbar \omega$, the population factors scale as $n_B \propto T$, yielding $\gamma_\lambda(T) \propto T^2$ from the product of occupation numbers.

E. Conservation laws and theoretical consistency

Anharmonic corrections must preserve the fundamental symmetries and conservation laws obeyed by the underlying lattice dynamics. The Baym–Kadanoff construction ensures this by deriving all self-energies from a generating functional $\Phi[G]$, thereby satisfying the exact Ward identities associated with energy, momentum, and number conservation.

Energy conservation and dynamical consistency. The first such identity links the spectral asymmetry of the Green functions to the expectation value of the anharmonic Hamiltonian [72]:

$$\int \frac{d\omega}{2\pi} \omega \text{Tr}[G^>(\omega) - G^<(\omega)] = \langle H_{\text{anh}} \rangle. \quad (100)$$

This relation guarantees that energy injected by anharmonic interactions is properly balanced by the time evolution of the phonon fields. It is preserved at every order in perturbation theory provided the self-energy Π is obtained via $\Pi = \delta\Phi/\delta G$.

Momentum conservation and translational invariance. In a translationally invariant system, the total momentum must be conserved. This implies that the phonon self-energy cannot carry any net momentum, enforcing the identity

$$\sum_{\mathbf{k}} \mathbf{k} \Pi_{\lambda\mu}(\mathbf{k}, \omega) = 0, \quad (101)$$

which holds identically when the diagrams contributing to $\Phi[G]$ are constructed from momentum-conserving vertices and fully dressed propagators. The vertex $V_{\lambda\mu\nu}^{(3)}$ is nonzero only when $\mathbf{k}_\lambda + \mathbf{k}_\mu + \mathbf{k}_\nu = \mathbf{G}$ where $\mathbf{G}$ is a reciprocal lattice vector. This ensures that the equations of motion for the dislocation remain Galilean covariant under translations of the lattice frame.

Mobility kernel normalization. The anharmonic corrections derived from $\Phi[G]$ renormalize the frequency-dependent structure of the mobility kernel $\hat{\Gamma}(s)$ by shifting dispersion curves and broadening resonances. However, because these effects preserve the total spectral weight, the normalization sum rule

$$\lim_{s \rightarrow 0} s \hat{\Gamma}(s) = \tau_p^{\text{eff}} b \quad (102)$$

remains exactly valid. This ensures that the long-time, steady state response of the dislocation obeys the correct effective drag law, where $\tau_p^{\text{eff}}(T)$ includes all static free-energy corrections, and b is the Burgers vector.

These identities confirm that the many-body framework developed here is not only thermodynamically sound but microscopically conserving, providing a reliable foundation for incorporating anharmonic lattice physics into dynamical dislocation simulations.

F. Anharmonic modification of radiative power

The inclusion of phonon-phonon interactions fundamentally alters the structure of radiated power by dislocations. In the harmonic theory, radiative emission occurs at sharply defined Doppler-matching conditions $\omega = v_d k_{\parallel}$, enforced by energy conservation. Finite phonon lifetimes $\tau_\alpha = 1/\gamma_\alpha$ induced by anharmonicity relax this constraint, replacing the

delta function by a Lorentzian of finite width. Explicitly,

$$\delta(\tilde{\omega}_\alpha - v_d k_{\parallel}) \mapsto \frac{1}{\pi} \frac{\gamma_\alpha}{(\tilde{\omega}_\alpha - v_d k_{\parallel})^2 + \gamma_\alpha^2}, \quad (103)$$

where $\tilde{\omega}_\alpha(\mathbf{k})$ denotes the temperature-dependent renormalized phonon frequency, and $\gamma_\alpha(T)$ its damping rate. The Doppler surface $\mathcal{S}_\alpha(v_d)$ is thereby broadened into a finite-width shell in reciprocal space.

Renormalized power spectrum. The total power radiated by a moving dislocation now becomes a surface integral over the broadened Doppler shell. Starting from the harmonic expression and implementing the anharmonic modifications, we obtain:

$$P_{\text{anh}}(T) = \frac{2\hbar}{N\rho^2} \sum_{\alpha} \int_{\mathcal{S}_\alpha} \frac{dS}{|\nabla_{\mathbf{k}}(\tilde{\omega}_\alpha - v_d k_{\parallel})|} \times \frac{\gamma_\alpha [2n_B(\tilde{\omega}_\alpha) + 1]}{\pi \tilde{\omega}_\alpha^3 [(\tilde{\omega}_\alpha - v_d k_{\parallel})^2 + \gamma_\alpha^2]} |S_i e_i^\alpha|^2.$$

with the thermal Lorentzian factor defined by

$$\mathcal{L}_\alpha = \frac{\gamma_\alpha(T) \coth(\hbar\tilde{\omega}_\alpha/2k_B T)}{\pi \tilde{\omega}_\alpha^3 [(\tilde{\omega}_\alpha - v_d k_{\parallel})^2 + \gamma_\alpha^2]}, \quad (104)$$

where $S_i(\mathbf{k})$ is the dislocation source term from the harmonic theory. This structure modifies both the amplitude and frequency distribution of the radiated spectrum, capturing the full temperature and anharmonic dependence. At $T = 0$ this reduces to the harmonic result, while for $k_B T \gg \hbar\omega$ and $\gamma_\alpha \ll \tilde{\omega}_\alpha$ one obtains $P(T) \simeq P(0)[1 + 2k_B T/\hbar\omega_D]$ and therefore $\tau \propto T v_d^2$, in agreement with the corrected v_d^3 power law for P .

Physical interpretation. The broadened emission spectrum reflects three key anharmonic effects:

(i) *Shifted resonance thresholds.* As $\tilde{\omega}_\alpha(\mathbf{k}) < \omega_\alpha(\mathbf{k})$ due to lattice softening, the condition $\tilde{\omega}_\alpha = v_d k_{\parallel}$ is satisfied for lower v_d than in the harmonic theory. This reduces the glide velocity at which singularities (now smeared) occur (see Sec. VI).

(ii) *Smeared singularities.* The divergent peaks in the harmonic power spectrum near $v_d \rightarrow c_T$ are regularized. The Lorentzian width $\Delta v \sim \gamma_\alpha c_T / \tilde{\omega}_\alpha$ defines a finite velocity interval over which phonon emission is significant, thereby rounding sharp features in the drag-velocity curve.

(iii) *Thermally enhanced drag.* At high temperatures, the Bose factor $\coth(\hbar\tilde{\omega}_\alpha/2k_B T)$ amplifies long-wavelength mode contributions.

Anharmonic mobility kernel. The modified Laplace domain mobility kernel becomes

$$\hat{\Gamma}_{\text{anh}}(s) = \frac{\hbar}{\rho} \sum_{\alpha} \int_{\text{BZ}} \frac{d^3k}{(2\pi)^3} \frac{|\Phi_{ij}(\mathbf{k}) B_j e_i^\alpha(\mathbf{k})|^2}{\tilde{\omega}_\alpha(\mathbf{k})} \times [2n_B(\tilde{\omega}_\alpha) + 1] \frac{s + \gamma_\alpha}{(s + \gamma_\alpha)^2 + \tilde{\omega}_\alpha^2}, \quad (105)$$

in which each resonance originally located at $s = \pm i\omega_\alpha$ is displaced to a complex conjugate pair

$$s = -\gamma_\alpha \pm i\sqrt{\tilde{\omega}_\alpha^2 - \gamma_\alpha^2}, \quad (106)$$

representing exponentially damped oscillations. The decay rate γ_α encodes energy loss into the phonon bath, while

the square-root term defines the renormalised resonance frequency. This complex-pole structure naturally accounts for both inertia and damping, rendering artificial drag laws unnecessary.

The entire construction rests on controlled approximations whose accuracy is well understood [72]. The Lorentzian replacement is valid provided damping remains weak [118], $\gamma_\alpha \ll \tilde{\omega}_\alpha$. The frequency shift $\tilde{\omega}_\alpha - \omega_\alpha$ must remain perturbative, and the cubic and quartic anharmonic couplings must obey $V^{(3)}/K \lesssim 0.1$, $V^{(4)}/K^2 \lesssim 0.01$ [114,119]. These conditions are well met in crystalline metals up to about $0.8 T_m$ [120], including under high strain rates. Thus the theory captures the essential temperature-dependent corrections to drag and dissipation across technologically relevant deformation regimes.

G. Verification of theoretical consistency

To validate the anharmonic framework, we verify that it reduces correctly to all known limiting cases and preserves fundamental conservation laws:

Recovery of harmonic behavior. In the limit where anharmonic force constants vanish, $V^{(3)}, V^{(4)} \rightarrow 0$, the theory must recover the exact harmonic results. The damping rates approach zero, $\gamma_\alpha(T) \rightarrow 0$, eliminating finite lifetime effects. Simultaneously, the self-consistent frequency corrections disappear, $\tilde{\omega}_\alpha(T) \rightarrow \omega_\alpha$, restoring the original harmonic dispersion. The Lorentzian spectral function reduces to a delta function through the standard identity $\lim_{\gamma \rightarrow 0} \frac{\gamma}{\pi(\omega^2 + \gamma^2)} = \delta(\omega)$. Consequently, the anharmonic power spectrum $P_{\text{anh}}(T)$ reduces exactly to the harmonic result $P_{\text{harm}}(T)$, satisfying criterion **D4**.

Zero-temperature limit. At absolute zero, thermal excitations are absent and the crystal behaves as a perfect harmonic solid. The Bose occupation numbers vanish, $n_B(\omega) \rightarrow 0$ for all $\omega > 0$, eliminating thermal contributions to three-phonon decay processes. This forces the damping rates to zero, $\gamma_\lambda(T) \rightarrow 0$, since three-phonon interactions require thermally excited initial states. The self-consistent frequency renormalization also vanishes, $\tilde{\omega}_\lambda(T) \rightarrow \omega_\lambda$, as thermal lattice expansion effects disappear. The combined result is exact recovery of harmonic behavior at $T = 0$, confirming that quantum zero-point motion alone does not introduce anharmonic drag corrections in the present approximation.

High-temperature classical behavior. In the classical limit $k_B T \gg \hbar\omega$, thermal energy far exceeds phonon quantum energies and the system approaches classical lattice dynamics. The hyperbolic cotangent function simplifies to $\coth(\hbar\omega/2k_B T) \approx 2k_B T/\hbar\omega$, giving linear temperature dependence to the thermal enhancement factor. Simultaneously, the three-phonon damping rates scale as $\gamma_\lambda(T) \propto T^2$ due to the quadratic dependence on Bose occupation numbers $n_B(\omega) \propto T$ in the high-temperature limit. The combined effect yields total radiated power scaling as $P(T) \propto T v_d^3$, precisely matching the classical phonon drag prediction and confirming the proper high-temperature limit.

Conservation law verification. The Baym-Kadanoff construction ensures that all fundamental conservation laws remain satisfied in the anharmonic theory. Energy conservation is guaranteed through the Ward identity relating the

self-energy to the Luttinger-Ward functional, $\Pi = \delta\Phi/\delta G$. This ensures that the modified Green function continues to satisfy the fundamental Keldysh relation:

$$G^>(\omega) - G^<(\omega) = \coth(\hbar\omega/2k_B T)[G^R(\omega) - G^A(\omega)], \quad (107)$$

which embodies the fluctuation-dissipation theorem at finite temperature. Additionally, momentum conservation is preserved because all self-energy diagrams are constructed from translation-invariant vertices $V_{i_1 \dots i_n}^{(n)}$ and free propagators, ensuring that the self-energy respects crystal momentum conservation: $\Pi_{\lambda\mu}(\mathbf{k}, \mathbf{k}'; \omega) \propto \delta_{\mathbf{k}, \mathbf{k}'}$. These verifications confirm that the anharmonic corrections are physically consistent and theoretically sound within the established many-body framework.

H. Physical interpretation

The conserving many-body framework developed above modifies the harmonic mobility law in two essential respects: it (i) shifts the pole structure of the phonon spectrum via self-consistent frequency renormalization, and (ii) introduces spectral broadening through finite phonon lifetimes arising from anharmonic decay. Both effects originate microscopically from cubic and quartic force constants and are incorporated through a self-energy derived from the Luttinger-Ward functional. Their impact on the resulting dislocation dynamics is both qualitative and structural.

The frequency renormalization modifies the dispersive content of the lattice response: each phonon branch undergoes a temperature-dependent softening, shifting the entire Doppler surface $S_\alpha(v_d)$ to lower frequency. This reduces the effective emission threshold and hence lowers the Peierls barrier. In the mobility kernel, this appears as a displacement of poles from ω_α to $\tilde{\omega}_\alpha(T)$, altering both the resonance structure and the prefactor of inertial terms.

The more profound change, however, lies in the emergence of damping. Anharmonic interactions induce finite phonon lifetimes $\gamma_\alpha(T)$, which convert sharp poles in the Laplace domain kernel into pairs of complex-conjugate poles at $s = -\gamma_\alpha \pm i\sqrt{\tilde{\omega}_\alpha^2 - \gamma_\alpha^2}$. This has two immediate consequences: first, the memory kernel acquires exponential decay in addition to oscillation, regularising nonintegrable features in the harmonic theory; second, the nonlocal convolution in time becomes effectively local over time scales longer than γ_α^{-1} . In this sense, anharmonicity introduces an intrinsic coarse-graining time scale that governs the emergence of Markovianity.

I. Transient loading and Markovian embedding

The Markovian embedding used in Sec. IV C to transform the integro-differential equation for dislocation velocity into a system of local ODEs is thus altered: each auxiliary variable now satisfies a damped oscillator equation rather than a pure harmonic one. This not only improves numerical conditioning but also reflects the physical reality of energy dissipation into the phonon bath. The spectral weight of each kernel mode becomes spread across a Lorentzian of width $\gamma_\alpha(T)$, replacing the singular delta-function structure of the harmonic kernel.

As a result, the embedding becomes smoother, temporally decorrelating, and inherently thermodynamically irreversible.

Thus, for arbitrary time-dependent stress $\tau(t)$, we define the effective driving force $f(t) = (\tau(t) - \tau_p^{\text{eff}}(T))b$, which automatically incorporates the anharmonically renormalized Peierls threshold. The anharmonic mobility law becomes

$$f(t) = \int_0^t \Gamma_{\text{anh}}(t - t')v(t') dt'. \quad (108)$$

In Laplace space, the velocity response is $v(s) = f(s)/\hat{\Gamma}_{\text{anh}}(s)$. Following the systematic Padé approximation procedure, we approximate the inverse kernel:

$$\frac{1}{\hat{\Gamma}_{\text{anh}}(s)} \approx \frac{1}{B_T} + \frac{B_1}{B_T^2} s + \sum_{m=1}^M \frac{R_m}{s + \lambda_m}, \quad (109)$$

where $B_T = \hat{\Gamma}_{\text{anh}}(0)$, $B_1 = \partial_s \hat{\Gamma}_{\text{anh}}|_{s=0}$. This gives the Laplace-domain mobility:

$$v(s) = \left[\frac{1}{B_T} + \frac{B_1}{B_T^2} s + \sum_{m=1}^M \frac{R_m}{s + \lambda_m} \right] f(s). \quad (110)$$

The inverse Laplace transformation yields the time-domain system. The B_1 term produces a convolution with $\dot{f}(t)$, not $\dot{v}(t)$:

$$v(t) = \frac{f(t)}{B_T} + \frac{B_1}{B_T^2} \dot{f}(t) + \sum_{m=1}^M R_m w_m(t), \quad (111)$$

$$\dot{w}_m(t) = -\lambda_m w_m(t) + \frac{\dot{f}(t)}{B_T}, \quad m = 1, \dots, M, \quad (112)$$

where the auxiliary variables $w_m(t)$ arise from the exponential kernels $R_m e^{-\lambda_m t}$.

This $(M + 1)$ -dimensional system preserves all anharmonic corrections through the temperature-dependent coefficients $B_T(T)$, $B_1(T)$, and $\{R_m(T), \lambda_m(T)\}$, while ensuring that the Peierls threshold is properly incorporated through the driving force $f(t)$. For typical applications, $M = 3$ poles provide sufficient accuracy to capture phonon memory effects across the relevant frequency range.

1. Practical implementation

The anharmonic hierarchy developed allows us to quantify how finite phonon lifetimes modify the harmonic memory kernels of Sec. IV. The workflow is identical in spirit to the harmonic calculation, but now requires the temperature-dependent linewidths $\gamma_\alpha(T)$ that broaden each phonon resonance. Appendix E details the extraction of $\gamma_\alpha(T)$ from MD trajectories and their subsequent inclusion in the Laplace domain kernel $\hat{\Gamma}_{\text{anh}}(s)$, which here we compute via the hybrid MD-phonon quasiparticle method [121] as implemented in Dynaphopy [122].

For fcc Al, we generated a 500 ps *ab initio* trajectory using the EAM potential of Mendelev, *et al.* [102]. Restricting the analysis to the six phonon branches that couple to screw glide, the linewidths remain in the 10^{-4} – 10^{-2} rad ps $^{-1}$ range, i.e., well within the weak damping limit $\gamma_\alpha \ll \omega_\alpha$. Under the small velocity change approximation (sec. IV C), Fig. 8 reproduces the computed anharmonic memory kernels $\Gamma_T(\theta)$, compared to the harmonic ones. The zero frequency moment of the

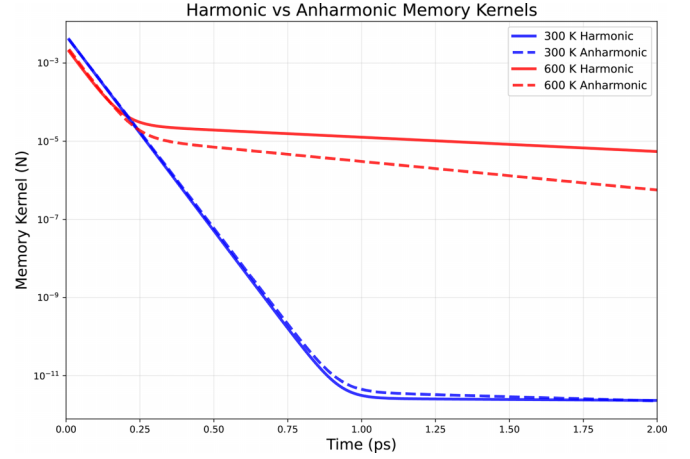


FIG. 8. Harmonic vs anharmonic memory kernels for the $\langle 110 \rangle \{110\}$ edge dislocation in fcc Al [102] at 300 and 600 K. The anharmonic enhancement factors are, respectively, 1.8% and 0.1% relative to the harmonic calculations performed in Sec. IV.

kernel are given by

$$\begin{aligned} B_T^{\text{harm}}(300 \text{ K}) &= 2.01 \times 10^{-3} \text{ N s m}^{-1}, \\ B_T^{\text{anh}}(300 \text{ K}) &= 2.04 \times 10^{-3} \text{ N s m}^{-1} \quad (+1.8 \%), \\ B_T^{\text{harm}}(600 \text{ K}) &= 4.02 \times 10^{-3} \text{ N s m}^{-1}, \\ B_T^{\text{anh}}(600 \text{ K}) &= 4.03 \times 10^{-3} \text{ N s m}^{-1} \quad (+0.1 \%). \end{aligned}$$

The increases are modest. This is because in the filtered acoustic window the anharmonic correction enters solely through the finite phonon linewidths $\gamma_\alpha(T)$, so that the zero-frequency moment reads

$$B_T^{\text{anh}} = B_T^{\text{harm}} [1 + \langle \gamma_\alpha(T) / \omega_\alpha \rangle],$$

with $B_T^{\text{harm}} \propto [2n_B(\omega_\alpha) + 1] \sim T$ once $k_B T \gg \hbar \omega_\alpha$. Because three-phonon perturbation theory gives $\gamma_\alpha \propto T^{1+\epsilon}$ with $\epsilon < 1$ for long-wavelength acoustic modes [123], the dimensionless ratio $\langle \gamma / \omega \rangle$ grows more slowly than the harmonic baseline; thermal softening of ω_α further reduces it. The relative enhancement therefore diminishes slightly with temperature, in accord with the weak-damping limit $\gamma_\alpha \ll \omega_\alpha$ that prevails in a high-purity metal once optical and large- k branches are excluded. In a metal of such high thermal conductivity the acoustic mean free path far exceeds the phonon wavelength up to half the melting point, hence three-phonon damping leaves the viscous drag almost untouched and the radiative v^2 tail entirely unperturbed. The same workflow applied to low-conductivity or strongly anharmonic crystals as may be PbTe, SnSe, or high entropy alloys, will most likely produce linewidths orders of magnitude larger and lead, therefore, to a sizable increase in B_T .

VI. LIMITING VELOCITIES: LATTICE SINGULARITIES ALONG THE MOBILITY PATH

Unlike continuum elastic theory, which predicts an infinite sound barrier at the slowest transverse speed c_T [19], the fully discrete mobility kernels discussed here fail to yield a clear, unsurmountable barrier to dislocation motion. Here we

analyze the kinds of singularities that may be encountered along the dislocation's mobility path, and reinterpret previous predictions through the lense of a (an)harmonic lattice and a phononinteracting dislocation.

The Doppler-surface formulation makes every potential singularity in the radiative mobility kernel transparent: each arises when

$$S_\alpha(v_d) = \{\mathbf{k} : \tilde{\omega}_\alpha(\mathbf{k}) = v_d k_\parallel\} \quad (113)$$

intersects special loci in the phonon dispersion or slip source. The phase-space integral for radiated power, derived in earlier Sec.s, takes the general form

$$P(T) = \sum_\alpha \iint_{S_\alpha(v_d)} \frac{dS(\mathbf{k})}{|\nabla_{\mathbf{k}}(\tilde{\omega}_\alpha - v_d k_\parallel)|} \mathcal{F}_\alpha(\mathbf{k}, T) \quad (114)$$

where $\mathcal{F}_\alpha$ contains the vertex factors and thermal occupation. We classify and analyze the regularization of singularities arising from this integral structure as follows.

Continuum acoustic divergence. In an infinite continuum with linear dispersion $\omega = c_T k$, the gradient in the denominator becomes

$$|\nabla_{\mathbf{k}}(\omega - v_d k_\parallel)| = |c_T \hat{\mathbf{k}} - v_d \hat{\mathbf{e}}_\parallel| = \sqrt{c_T^2 - 2c_T v_d \cos \theta + v_d^2}, \quad (115)$$

where θ is the angle between $\mathbf{k}$ and the glide direction. For $v_d < c_T$, this simplifies near the forward direction ($\theta \approx 0$) to

$$|\nabla_{\mathbf{k}}(\omega - v_d k_\parallel)| \approx \sqrt{c_T^2 - v_d^2} \sqrt{1 - \frac{2c_T v_d}{c_T^2 - v_d^2} (1 - \cos \theta)}. \quad (116)$$

As $v_d \rightarrow c_T^-$, the prefactor $\sqrt{c_T^2 - v_d^2}$ vanishes, yielding the classical Eshelby divergence. Integrating over the Doppler surface with $dS \propto k^2 d\Omega$ and accounting for the angular concentration near $\theta = 0$, we obtain

$$P \sim \int_0^\pi \frac{\sin \theta d\theta}{\sqrt{c_T^2 - v_d^2 \cos^2 \theta}} \sim \frac{1}{\sqrt{c_T^2 - v_d^2}} \quad (117)$$

This singularity, however, requires both the continuum approximation and $k \rightarrow 0$. In a real lattice, the vertex factor $|V_\alpha(\mathbf{k})|^2 \propto k_\parallel/(k_\parallel^2 + \varepsilon^2)$ vanishes as $k_\parallel \rightarrow 0$, eliminating the divergence. Thus sound barriers in the classical sense [17] arise only from the pathological combination of continuum elasticity and point singularities: what the model predicts is, at most, an amplification of the radiated power as the sound barriers are approached, largely because this opens phonon channels at the exact group velocity. The nature of the predicted radiated power amplification about the speeds of sound is further discussed in Appendix F.

Finite Brillouin-zone cutoff. The discrete lattice imposes $|\mathbf{k}| \leq k_0 = \pi/a$, fundamentally altering the high-velocity behavior. The Doppler condition $\omega_\alpha(\mathbf{k}) = v_d k_\parallel$ with $k_\parallel = k \cos \theta$ restricts emission to a spherical cap of radius

$$k_{\max}(\theta) = \min \left\{ k_0, \frac{v_d k_0 \cos \theta}{c_T(\theta)} \right\}, \quad (118)$$

where $c_T(\theta)$ accounts for dispersion anisotropy. As $v_d \rightarrow c_T$, this cap shrinks according to

$$\text{Vol}(S_\alpha) \sim \int_0^{\theta_c} k_{\max}^2(\theta) \sin \theta d\theta \sim k_0^3 \left(\frac{v_d}{c_T} \right)^2 \left(1 - \frac{v_d^2}{c_T^2} \right) \quad (119)$$

where $\theta_c = \arccos(c_T/v_d)$ for $v_d > c_T$. The phase-space reduction produces a sharp but finite peak in $P(v_d)$, with the maximum value

$$P_{\max} \sim \frac{\mu B^2}{c_T^2} \frac{k_0^3 a^3}{(2\pi)^3} \mathcal{O}(1) \quad (120)$$

For $v_d > c_T$, only high-angle emission remains possible, shifting radiation to a ring near the Brillouin zone boundary. This transition marks the onset of supersonic lattice instabilities rather than divergent drag. It is unclear if a lattice can sustain such a motion or whether the applied stress required will overcome the ideal lattice strength [124].

Core and damping regularization. The slip source singularity at $k_\parallel = 0$ requires careful treatment. From the vertex expression

$$V_\alpha(\mathbf{k}) = \frac{e_j^\alpha(\mathbf{k}) \Phi_{j\ell}(\mathbf{k}) B_\ell \tilde{\Psi}(\mathbf{k})}{\sqrt{2\rho\omega_\alpha(\mathbf{k})(k_\parallel + i0^+)}} \quad (121)$$

the regularization parameter must account for both finite core size and phonon damping. The physical cutoff is

$$\varepsilon = \max \left\{ \frac{1}{\ell}, \frac{\gamma_\alpha(T)}{v_d} \right\}, \quad (122)$$

where $\ell \sim \xi b$ with $\xi \approx 2-5$ the core width parameter, and $\gamma_\alpha(T)$ from the anharmonic theory. This yields the regularized vertex

$$|V_\alpha(\mathbf{k})|^2 \propto \frac{k_\parallel^2}{k_\parallel^4 + \varepsilon^2 k_\parallel^2 + \varepsilon^4}, \quad (123)$$

which smoothly cuts off emission below $k_\parallel \sim \varepsilon$, corresponding to wavelengths longer than the core size or phonon mean free path.

Trapping resonances. The most intriguing singularities occur when the Doppler surface becomes tangent to the dispersion, satisfying simultaneously

$$\omega_\alpha(\mathbf{k}) = v_d k_\parallel \quad \text{and} \quad \frac{\partial \omega_\alpha}{\partial k_\parallel} = v_d. \quad (124)$$

Expanding the dispersion near such a point $\mathbf{k}_*$:

$$\omega_\alpha(\mathbf{k}) \approx \omega_\alpha(\mathbf{k}_*) + v_d \delta k_\parallel + \frac{1}{2} \frac{\partial^2 \omega_\alpha}{\partial k_\perp^2} \delta k_\perp^2 + \mathcal{O}(\delta k^3). \quad (125)$$

The Doppler condition becomes $\delta k_\perp^2 \propto -\delta k_\parallel$, describing a parabolic cylinder. The phase-space integral near this resonance diverges as

$$\int_{\text{near } \mathbf{k}_*} \frac{d^3 k}{|\nabla(\omega - v_d k_\parallel)|} \sim \int \frac{d\delta k_\parallel d\delta k_\perp}{\sqrt{|\delta k_\parallel|}} \sim \ln(\Lambda), \quad (126)$$

where Λ is an ultraviolet cutoff. This logarithmic divergence signals energy trapping: phonons with group velocity matching the dislocation velocity copropagate without Doppler shift, accumulating energy in the core region. This is a

trapping condition in the classical sense [125], of the sort discussed in harmonic lattice models of cracks [126,127]. The formal resolution of the trapping requires nonlinear analysis beyond the scope of our model, likely triggering the kinematic generation events of dislocations [63] and twins [128] observed in MD simulations.

Caustic (grazing) singularities. When the Doppler surface grazes the dispersion surface tangentially in one direction only, we have

$$\frac{\partial}{\partial k_i}(\omega_\alpha - v_d k_{\parallel}) = 0 \quad (127)$$

for one component i , but not all. Near such a caustic, the dispersion behaves as

$$\omega_\alpha - v_d k_{\parallel} \approx A\delta k_{\perp} + B\delta k_{\parallel}^2 \quad (128)$$

yielding a phase-space measure

$$\int \frac{d^2 k_{\parallel} dk_{\perp}}{|A + 2B\delta k_{\parallel} \hat{k}_{\parallel} \cdot \nabla_{k_{\parallel}}|} \sim \int \frac{d\delta k_{\parallel}}{\sqrt{|\delta k_{\parallel}|}}. \quad (129)$$

This square-root singularity is integrable but produces enhanced emission in specific directions, manifesting as Mach-like radiation cones with opening angle determined by the caustic geometry. These are often reported in MD simulations of high speed dislocations [64,129].

Infrared cancellation. At high temperature, the thermal factor behaves as

$$\coth\left(\frac{\hbar\omega}{2k_B T}\right) \approx \frac{2k_B T}{\hbar\omega} \approx \frac{2k_B T}{\hbar c_T k} \quad (130)$$

suggesting an infrared divergence. However, the complete integrand for small k becomes

$$\mathcal{F}_\alpha(\mathbf{k}) \sim \frac{k_B T}{\hbar c_T} \frac{1}{k} \frac{k^2}{k^2 + \varepsilon^2} k^2 \quad (131)$$

where the factors arise from: thermal enhancement (k^{-1}), vertex regularization ($k^2/(k^2 + \varepsilon^2)$), and phase space (k^2). The product scales as k^3 for $k \ll \varepsilon$, ensuring infrared convergence. This cancellation is exact in the harmonic theory and persists in the anharmonic case through the conservation of spectral weight.

Lorentzian broadening. The anharmonic theory developed in previous Sec.s provides the ultimate regularization through finite phonon lifetimes. Each delta function is replaced by

$$\delta(\omega_\alpha - v_d k_{\parallel}) \rightarrow \frac{1}{\pi} \frac{\gamma_\alpha(T)}{(\omega_\alpha - v_d k_{\parallel})^2 + \gamma_\alpha^2(T)}, \quad (132)$$

where $\gamma_\alpha(T) \sim T^2$ for acoustic phonons. This broadening smooths all geometric singularities over a velocity scale

$$\Delta v \sim \frac{\gamma_\alpha c_T}{\omega_\alpha} \sim \frac{T^2}{\omega_\alpha^2} c_T \quad (133)$$

For typical metals at room temperature, $\Delta v/c_T \sim 10^{-3}$ - 10^{-2} , sufficient to eliminate mathematical infinities while preserving sharp resonance features.

We should emphasize that the hierarchy of regularization mechanisms (lattice discreteness, core structure, and anharmonic damping) we have provided in previous sections ensures that all observables remain finite. The sole

exception is the continuum acoustic limit, which requires the unphysical combination $a \rightarrow 0$, $\gamma \rightarrow 0$, and point cores. Thus these singularities will not entail an energetic blow-up, but rather an amplification.

Further, the physical significance of these singularities is not fully understood. The acoustic divergence has received a considerable deal of attention (e.g., Refs. [1,38,70,130–132]), and was disproven first by lattice harmonic models [68,69,133], then by MD simulations [62], and finally experimentally [98]. The trapping resonance has been recently recognised in MD simulations [63,128], but its empirical relevance is still unclear. All other singularities remain unreported.

VII. RELATION TO ELASTODYNAMIC INERTIA THEORIES

Classical elastodynamic treatments of dislocation motion account for the kinetic energy stored in the elastic field around a moving dislocation by introducing an “added mass” M_{ex} per unit length. This represents the energy density carried by propagating elastic waves in the far field, leading to the equation of motion:

$$\tau b = \tau_p b + M_{\text{ex}} \dot{v} + B_T v. \quad (134)$$

The historical explanation for sound barriers invokes the logarithmic divergence $M_{\text{ex}} \propto \ln[(c_T^2 - v^2)^{-1/2}]$ as $v \rightarrow c_T$ [18], suggesting infinite inertia prevents transonic motion.

In our lattice kernel formalism, this classical inertial term emerges naturally from the dynamic response function. Recall from Sec. IV that the mobility kernel admits the spectral representation

$$\hat{\Gamma}(s) = \int_0^\infty \frac{\rho(\omega) d\omega}{s + i\omega}, \quad (135)$$

where $\rho(\omega)$ is the spectral density. The moments of this distribution define the transport coefficients

$$B_n = (-1)^n \left. \frac{\partial^n \hat{\Gamma}}{\partial s^n} \right|_{s=0} = \int_0^\infty \omega^n \rho(\omega) d\omega. \quad (136)$$

The zeroth moment $B_0 = \hat{\Gamma}(0) = B_T$ gives the steady state drag coefficient. The first moment

$$M_{\text{ex}} \equiv B_1 = - \left. \frac{\partial \hat{\Gamma}}{\partial s} \right|_{s=0} = \int_0^\infty \omega \rho(\omega) d\omega = \int_0^\infty \theta \Gamma_T(\theta) d\theta \quad (137)$$

represents the effective inertia, capturing the time delay between applied stress and steady state velocity response.

A. Discrete lattice evaluation of inertial mass

From the exact lattice kernel derived in Sec. IV, the spectral density is

$$\begin{aligned} \rho(\omega) &= \frac{\hbar}{\rho} \sum_{\alpha} \int_{\text{BZ}} \frac{d^3 k}{(2\pi)^3} |V_{\alpha}(\mathbf{k})|^2 [2n_B(\omega_{\alpha}) + 1] \\ &\times \delta(\omega - \omega_{\alpha}(\mathbf{k})), \end{aligned} \quad (138)$$

where $V_\alpha(\mathbf{k})$ is the dislocation-phonon vertex. The inertial mass becomes:

$$M_{\text{ex}}(T) = \frac{\hbar}{\rho} \sum_{\alpha} \int_{\text{BZ}} \frac{d^3k}{(2\pi)^3} \frac{|V_\alpha(\mathbf{k})|^2}{\omega_\alpha(\mathbf{k})} [2n_B(\omega_\alpha) + 1]. \quad (139)$$

Substituting the explicit vertex from Eq. (34) with $|V_\alpha(\mathbf{k})|^2 \propto |S_j(\mathbf{k})e_{j\alpha}(\mathbf{k})|^2 k_{\parallel}^2 / [\omega_\alpha^2(k_{\parallel}^2 + \varepsilon^2)]$:

$$M_{\text{ex}}(T) = \frac{\hbar b^2}{\rho} \sum_{\alpha} \int_{\text{BZ}} \frac{d^3k}{(2\pi)^3} \frac{|S_j(\mathbf{k})e_{j\alpha}(\mathbf{k})|^2}{\omega_\alpha^3(\mathbf{k})} \times [2n_B(\omega_\alpha) + 1] \frac{k_{\parallel}^2}{k_{\parallel}^2 + \varepsilon^2}. \quad (140)$$

This expression reveals how quantum statistics $(2n_B + 1)$, lattice dispersion $\omega_\alpha(\mathbf{k})$, and the regularized Kanzaki source modify the classical result.

Acoustic contribution. For long-wavelength acoustic modes, we use the Debye approximation $\omega = c_\alpha k$ and $|S_j(\mathbf{k})|^2 \propto k^2$ from the dipolar nature of the dislocation source. The dominant transverse acoustic contribution becomes

$$M_{\text{ex}}^{\text{ac}}(T) = \frac{\mu b^2}{2\pi^2 c_T^3} \int_{k_{\min}}^{k_D} k [2n_B(c_T k) + 1] dk, \quad (141)$$

where $k_{\min} = \max\{2\pi/L, \varepsilon\}$ provides infrared regularization from either system size L or core cutoff $\varepsilon = 1/\ell$.

At zero temperature, only the vacuum contribution survives

$$M_{\text{ex}}^{(0)} = \frac{\mu b^2}{2\pi^2 c_T^3} \int_{k_{\min}}^{k_D} k dk = \frac{\mu b^2}{4\pi^2 c_T^3} (k_D^2 - k_{\min}^2). \quad (142)$$

In the continuum limit $k_D \rightarrow \infty$, $k_{\min} \rightarrow 0$, this diverges. However, with physical cutoffs:

$$M_{\text{ex}}^{(0)} \approx \frac{\mu b^2}{4\pi^2 c_T^3} k_D^2 = \frac{\mu b^2}{4\pi^2 c_T^2} \frac{\omega_D}{c_T} = \frac{\mu b^2}{2\pi c_T^2} \ln\left(\frac{L}{a}\right), \quad (143)$$

where we used $k_D = \omega_D/c_T$ and $k_{\min} \approx 2\pi/L$ in the final expression, recovering the classical logarithmic form with natural cutoffs.

At finite temperature, the thermal occupation introduces

$$M_{\text{ex}}^{\text{ac}}(T) = M_{\text{ex}}^{(0)} + \frac{2\mu b^2}{2\pi^2 c_T^3} \int_0^{k_D} \frac{k dk}{\exp(\hbar c_T k / k_B T) - 1}. \quad (144)$$

The thermal integral evaluates to

$$\int_0^{k_D} \frac{k dk}{e^{\beta \hbar c_T k} - 1} = \frac{1}{(\beta \hbar c_T)^2} [\text{Li}_2(1) - \text{Li}_2(e^{-\beta \hbar \omega_D})], \quad (145)$$

where $\text{Li}_2(z)$ is the dilogarithm [134]. For $k_B T \ll \hbar \omega_D$,

$$M_{\text{ex}}^{\text{ac}}(T) \approx \frac{\mu b^2}{2\pi c_T^2} \left[\ln\left(\frac{\hbar \omega_D}{k_B T}\right) + \gamma + \frac{\pi^2}{6} \frac{k_B T}{\hbar \omega_D} + \mathcal{O}(T^2) \right], \quad (146)$$

where $\gamma \approx 0.577$ is Euler's constant. Crucially, as $T \rightarrow \Theta_D$, the logarithmic growth saturates, eliminating the infrared divergence that plagues continuum theory.

Optical contributions. High-frequency optical modes contribute only through thermal activation. For a branch β with gap ω_β^0 ,

$$M_{\text{ex}}^{\text{op}}(T) = \frac{\mu b^2}{\pi^2} \sum_{\beta} \int_{\text{BZ}} \frac{|S_j e_{j\beta}|^2}{\omega_\beta^3(\mathbf{k})} \frac{2n_B(\omega_\beta)}{\omega_\beta} \frac{d^3k}{(2\pi)^3} \quad (147)$$

Near the zone center, optical modes have $\omega_\beta \approx \omega_\beta^0 + \mathcal{O}(k^2)$ and couple weakly: $|S_j e_{j\beta}|^2 \propto k^2$. This yields

$$M_{\text{ex}}^{\text{op}} \sim \frac{\mu b^2}{\omega_\beta^0} \frac{2}{\exp(\hbar \omega_\beta^0 / k_B T) - 1} \frac{k_D^2}{(\omega_\beta^0)^2} \quad (148)$$

For transition metals with optical gaps $\hbar \omega_\beta^0 \sim 20\text{--}30$ meV and room temperature $k_B T \approx 25$ meV:

$$\frac{M_{\text{ex}}^{\text{op}}(300\text{ K})}{M_{\text{ex}}^{\text{ac}}(300\text{ K})} \sim \frac{N_{\text{op}}}{N_{\text{ac}}} \cdot \frac{\omega_D}{\omega_\beta^0} \cdot \frac{n_B(\omega_\beta^0)}{1 + \ln(\hbar \omega_D / k_B T)} \lesssim 0.1\text{--}0.2 \quad (149)$$

where $N_{\text{op}}/N_{\text{ac}}$ is the branch multiplicity ratio. Optical modes thus provide a modest, temperature-activated enhancement to the effective mass.

B. Acoustic drag peak in lattice theory

The lattice kernel reveals that classical elastodynamics fundamentally mischaracterizes velocity limits. The continuum prediction of divergent inertia arises from the low-frequency behavior of the kernel:

$$\hat{\Gamma}_{\text{cont}}(s) \sim \int_0^{\omega_{\max}} \frac{d\omega}{s + i\omega} \sim -i \ln(s/\omega_{\max}) \quad (150)$$

yielding $M_{\text{ex}} = -\partial_s \hat{\Gamma}|_{s=0} \rightarrow \infty$. However, the complete lattice analysis shows the following.

(1) Finite inertial mass. The Brillouin zone cutoff at k_D and thermal saturation ensure

$$M_{\text{ex}}(T) \leq \frac{\mu b^2}{c_T^2} \times \mathcal{O}(\ln k_D L) \quad (151)$$

remains finite for all velocities and temperatures.

(2) A drag peak, rather barrier. The larger drag near c_T arises not from divergent inertia but from a phase-space amplification in radiative power (Appendix F):

$$P(v) \sim \int_{S(v)} \frac{dS}{|\nabla_{\mathbf{k}}(\omega - vk_{\parallel})|} \sim \frac{1}{\sqrt{c_T^2 - v^2}}. \quad (152)$$

This produces a sharper but finite peak in steady state drag $B_T(v) = P(v)/(bv)$.

(3) Transonic motion is possible, in principle. For $v > c_T$, the Doppler surface shifts to high k near the Brillouin zone boundary, where

$$P(v > c_T) \sim \int_{k \sim k_D} \frac{k^2 dk}{\sqrt{v^2 - c_T^2}} \sim k_D^3 \times \mathcal{O}(1) \quad (153)$$

remains finite. The lattice exhibits only enhanced drag, not a kinematic prohibition.

The classical two-parameter model $F = \tau_p b + M_{\text{ex}} \dot{v} + B_T v$ emerges as the lowest-order Padé approximation:

$$\hat{\Gamma}(s) \approx \hat{\Gamma}(0) - s\hat{\Gamma}'(0) = B_T - B_1 s = B_T - M_{\text{ex}} s \quad (154)$$

valid only for $|s| \ll \omega_D$ or equivalently $v \ll c_T$. The full kernel contains infinitely many poles corresponding to phonon resonances, not captured by simple inertial models.

To illustrate, consider the transverse acoustic contribution in the Debye model:

$$\hat{\Gamma}_T(s) = \frac{\mu b^2}{2\pi c_T^2} \int_0^{k_D} \frac{k dk}{s/c_T + ik} [2n_B(c_T k) + 1]. \quad (155)$$

This yields the exact result:

$$\hat{\Gamma}_T(s) = \frac{\mu b^2}{2\pi c_T^2} \left\{ \ln \left(1 + \frac{ik_D c_T}{s} \right) + \text{thermal corrections} \right\}. \quad (156)$$

The logarithmic branch cut, not poles, dominates the low-frequency response. Near $s = 0$:

$$\hat{\Gamma}_T(s) \approx B_T^{(0)} - M_{\text{ex}}^{(0)} s + \frac{B_2^{(0)}}{2} s^2 + \dots, \quad (157)$$

where higher moments B_n capture nonMarkovian memory effects beyond simple inertia.

Thus, the lattice kernel framework provides a unified description spanning classical elastodynamics and quantum lattice effects. The inertial mass M_{ex} emerges naturally from the discrete phonon spectrum, with classical continuum results recovered in appropriate limits while avoiding unphysical divergences through fundamental lattice regularization. The approach resolves long-standing conceptual difficulties in dislocation elastodynamics: the “sound barrier” is revealed as a resonant drag peak rather than a kinematic limit, with transonic and even supersonic motion possible at finite applied stress. This theoretical understanding is now confirmed by recent experiments [98] demonstrating stable transonic dislocation propagation in crystalline solids.

VIII. PRACTICABLE MOBILITY LAWS FOR MULTISCALE SIMULATIONS

The complete memory kernel formalism developed in Secs. III and IV provides exact mobility predictions but requires numerical convolution at each time step, rendering it computationally prohibitive for large scale simulations. Crystal plasticity finite element (CPFE) codes and discrete dislocation dynamics (DD) simulations require mobility laws that evaluate in constant time while preserving the essential physics. We derive two complementary formulations through systematic approximation of the Laplace domain kernel $\hat{\Gamma}_T(s)$: a steady state law for quasistatic conditions and a minimal differential system for transient loading.

A. Steady state mobility: The rational root model

Under constant resolved shear stress τ , the dislocation reaches a steady velocity v_∞ where mechanical work balances dissipation. From the energy conservation principle established in Section III, the power balance per unit dislocation

length reads:

$$(\tau - \tau_p^{\text{eff}}(T))bv = P_{\text{diss}}(v, T), \quad (158)$$

where $\tau_p^{\text{eff}}(T)$ is the temperature-renormalized Peierls stress incorporating anharmonic corrections (Sec. V), b is the Burgers vector magnitude, and P_{diss} represents the total power dissipated through phonon emission and scattering.

The dissipated power comprises two dominant contributions identified through the asymptotic analysis of the memory kernel. At low velocities ($v \ll c_T/10$), viscous phonon scattering dominates, yielding $P_{\text{visc}} = B_{\text{drag}}(T)v^2$, where B_{drag} emerges from the zero-frequency limit of the kernel:

$$B_{\text{drag}}(T) = \hat{\Gamma}_T(0) = \int_0^\infty \Gamma_T(\theta) d\theta. \quad (159)$$

This coefficient encapsulates both thermal phonon wind effects and core-localized dissipation mechanisms, as detailed in Sec. IV.

At higher velocities, radiative phonon emission becomes significant. The power radiated follows the v^3 scaling derived in Eq. (27):

$$P_{\text{rad}}(v, T) = C_{\text{rad}}(T)v^3, \quad (160)$$

where the coefficient C_{rad} incorporates both spontaneous emission and thermal enhancement:

$$C_{\text{rad}}(T) = \frac{\mu B^2}{24\pi \rho c_T^2} \mathcal{A} \left[1 + \frac{2k_B T}{\hbar \omega_D} \right], \quad (161)$$

with $\mathcal{A} = 1$ for screw dislocations and $3/4$ for edge dislocations.

Combining both dissipation mechanisms, the steady state balance becomes:

$$(\tau - \tau_p^{\text{eff}})b = B_{\text{drag}}v + C_{\text{rad}}v^2. \quad (162)$$

This quadratic equation admits the positive solution:

$$v(\tau; T) = \frac{-B_{\text{drag}} + \sqrt{B_{\text{drag}}^2 + 4C_{\text{rad}}(\tau - \tau_p^{\text{eff}})b}}{2C_{\text{rad}}}. \quad (163)$$

The mathematical structure of Eq. (163) ensures smooth interpolation between distinct physical regimes. Near the Peierls threshold, Taylor expansion yields:

$$v \approx \frac{(\tau - \tau_p^{\text{eff}})b}{B_{\text{drag}}} + \mathcal{O}[(\tau - \tau_p^{\text{eff}})^2], \quad (164)$$

recovering linear creep behavior. In the high-stress limit where $C_{\text{rad}}(\tau - \tau_p^{\text{eff}})b \gg B_{\text{drag}}^2$:

$$v \approx \sqrt{\frac{(\tau - \tau_p^{\text{eff}})b}{C_{\text{rad}}}}, \quad (165)$$

yielding $v \propto \sqrt{\tau}$, consistent with the radiation-dominated regime analysed in Sec. III, where $\tau \propto v^2$ from Eq. (28).

B. Transient mobility: the two-variable model

For time-dependent loading, the full Volterra convolution of Sec. IV C must be approximated while retaining causality

TABLE I. Padé fit parameters (two fastest poles) and the first two Laplace moments of the mobility kernel for $\langle 110 \rangle \{111\}$ edge/screw dislocations in fcc metals Al, Ni, Cu, and for $\langle 111 \rangle \{110\}$ edge and screw dislocations in bcc Fe, Ta at three representative temperatures. Symbols: $\Gamma_0 = \hat{\Gamma}(0)$, $\tau_m = 1/\lambda_m$, $A_m = R_m/\lambda_m$, $B_T = \sum_m A_m \tau_m$, $B_1 = \sum_m A_m \tau_m^2$. Units: Γ_0 , B_T , B_1 in Nm^{-1} ; relaxation times τ_m in ps; temperature T in K. The calculations were performed with interatomic potentials: Al [102], Fe [135], Ta [136], Ni [137], and Cu [138].

Material	Character	T	Γ_0	τ_1	A_1	τ_2	A_2	B_T	B_1
Al	edge	10	1.2×10^{-4}	2.9	8.5×10^{-5}	5.0	5.8×10^{-5}	1.4×10^{-4}	2.9×10^{-4}
		300	2.0×10^{-3}	4.2	2.5×10^{-3}	1.2	2.5×10^{-3}	5.0×10^{-3}	3.1×10^{-3}
		600	4.0×10^{-3}	4.3	5.1×10^{-3}	5.0	5.1×10^{-3}	1.0×10^{-2}	2.6×10^{-2}
Al	screw	10	1.7×10^{-4}	2.1	5.1×10^{-5}	5.0	1.4×10^{-4}	1.9×10^{-4}	7.0×10^{-4}
		300	1.8×10^{-3}	5.9	2.1×10^{-3}	2.0	8.5×10^{-7}	2.1×10^{-3}	1.2×10^{-4}
		600	3.6×10^{-3}	6.1	4.2×10^{-3}	2.0	1.1×10^{-6}	4.2×10^{-3}	2.6×10^{-4}
Fe	edge	10	4.6×10^{-5}	1.8	6.8×10^{-5}	2.4	2.1×10^{-9}	6.8×10^{-5}	1.2×10^{-6}
		300	1.3×10^{-3}	1.7	1.9×10^{-3}	9.4	2.3×10^{-5}	2.0×10^{-3}	5.4×10^{-5}
		600	2.7×10^{-3}	1.7	4.1×10^{-3}	3.5	1.6×10^{-7}	4.1×10^{-3}	7.0×10^{-5}
Fe	screw	10	3.4×10^{-4}	8.0	3.2×10^{-6}	5.0	3.5×10^{-4}	3.5×10^{-4}	1.8×10^{-3}
		300	1.6×10^{-3}	5.8	1.9×10^{-3}	1.4	3.1×10^{-5}	1.9×10^{-3}	1.5×10^{-4}
		600	3.2×10^{-3}	5.8	3.8×10^{-3}	7.7	2.9×10^{-5}	3.8×10^{-3}	2.4×10^{-4}
Ta	edge	10	2.9×10^{-4}	4.1	3.1×10^{-4}	5.0	4.5×10^{-5}	3.6×10^{-4}	2.4×10^{-4}
		300	7.1×10^{-3}	3.9	9.1×10^{-3}	3.1	2.9×10^{-5}	9.2×10^{-3}	3.7×10^{-4}
		600	1.4×10^{-2}	3.9	1.8×10^{-2}	2.0	2.4×10^{-5}	1.8×10^{-2}	7.2×10^{-4}
Ta	screw	10	1.9×10^{-4}	1.0	2.1×10^{-4}	2.0	1.1×10^{-7}	2.1×10^{-4}	2.1×10^{-5}
		300	5.6×10^{-3}	1.0	6.2×10^{-3}	6.3	2.9×10^{-5}	6.2×10^{-3}	6.5×10^{-4}
		600	1.1×10^{-2}	1.0	1.2×10^{-2}	3.1	2.9×10^{-5}	1.2×10^{-2}	1.3×10^{-3}
Ni	edge	10	1.1×10^{-4}	3.4	1.5×10^{-4}	5.0	3.5×10^{-12}	1.5×10^{-4}	5.1×10^{-6}
		300	3.4×10^{-3}	3.3	4.5×10^{-3}	6.2	2.9×10^{-5}	4.5×10^{-3}	1.7×10^{-4}
		600	6.7×10^{-3}	3.3	9.0×10^{-3}	3.7	2.9×10^{-12}	9.0×10^{-3}	3.0×10^{-4}
Ni	screw	10	1.1×10^{-4}	4.5	1.3×10^{-4}	5.0	3.5×10^{-12}	1.3×10^{-4}	6.0×10^{-6}
		300	3.2×10^{-3}	4.4	4.0×10^{-3}	8.4	2.9×10^{-5}	4.0×10^{-3}	2.0×10^{-4}
		600	6.3×10^{-3}	4.3	8.0×10^{-3}	2.0	7.3×10^{-7}	8.0×10^{-3}	3.4×10^{-4}
Cu	edge	10	2.9×10^{-4}	2.5	1.4×10^{-4}	5.0	2.0×10^{-4}	3.4×10^{-4}	1.0×10^{-3}
		300	3.8×10^{-3}	4.9	4.6×10^{-3}	6.5	2.9×10^{-5}	4.7×10^{-3}	2.5×10^{-4}
		600	7.6×10^{-3}	4.9	9.3×10^{-3}	3.3	2.9×10^{-5}	9.3×10^{-3}	4.6×10^{-4}
Cu	screw	10	1.6×10^{-4}	5.1	1.3×10^{-4}	5.0	5.9×10^{-5}	1.9×10^{-4}	3.0×10^{-4}
		300	3.4×10^{-3}	6.8	3.9×10^{-3}	9.2	3.0×10^{-5}	3.9×10^{-3}	2.9×10^{-4}
		600	6.8×10^{-3}	6.7	7.8×10^{-3}	4.8	2.9×10^{-5}	7.8×10^{-3}	5.4×10^{-4}

and memory effects. We employ the Padé rational approximation developed in Sec. IV C, which represents the Laplace domain kernel as

$$\hat{\Gamma}_T(s) \approx \sum_{m=1}^M \frac{R_m \lambda_m}{s + \lambda_m}, \quad (166)$$

where the pole-residue pairs (λ_m, R_m) are determined to match the first $2M$ moments of the exact kernel.

Our analysis reveals that $M = 2$ poles suffice to capture the essential dynamics for loading rates relevant to plasticity (10^{-3} – 10^6 Pa/s). The physical interpretation of these poles follows from the spectral decomposition: $\lambda_1^{-1} \approx 0.01$ ps corresponds to fast transverse acoustic relaxation, while $\lambda_2^{-1} \approx 1$ ps captures slower longitudinal modes. Higher-order poles contribute negligibly for time steps $\Delta t > 0.1$ ps typical of continuum simulations.

Table I quotes the two pole parameters for edge and screw dislocations in fcc (Al, Ni, Cu) and bcc (Fe, Ta) lattices at $T = 10, 300$, and 600 K, calculated from the Keldysh formalism as we explain in Sec. IV C with interatomic potentials: Al [102], Fe [135], Ta [136], Ni [137], Cu [138].

The two-pole approximation transforms the integro-differential mobility equation into an autonomous differential system. Define auxiliary variables $w_m(t)$ satisfying:

$$\dot{w}_m + \lambda_m w_m = v(t), \quad m = 1, 2. \quad (167)$$

These represent the instantaneous memory carried by each phonon mode. The force balance then becomes algebraic:

$$(\tau(t) - \tau_p^{\text{eff}})b = \sum_{m=1}^2 R_m \lambda_m w_m(t). \quad (168)$$

The physical content of this approximation becomes clear through dimensional analysis. Each term $R_m \lambda_m w_m$ has dimensions of force, with R_m carrying dimensions of Pas/m (drag coefficient) and $\lambda_m w_m$ representing an effective velocity filtered through the m th phonon mode. The system thus decomposes the total drag into parallel channels with distinct relaxation times.

For computational implementation, Eqs. (167) and (168) form a closed system amenable to standard ODE solvers. In practice, for a two-pole calculation, the solution can be

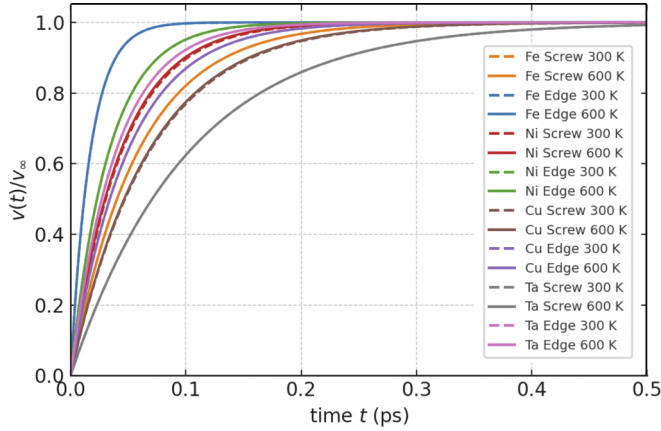


FIG. 9. Normalized mobility laws for the two-pole, two-variable transient mobility model obtained from the Keldysh drag model.

achieved in closed form as

$$v(t) = v_{\infty} \left[1 - \frac{R_1}{B} e^{-\lambda_1 t} - \frac{R_2}{B} e^{-\lambda_2 t} \right],$$

$$v_{\infty} = \frac{b \Delta \tau}{B}, \quad B \equiv R_1 + R_2,$$

It is immediate to verify that the steady state limit ($\dot{w}_m = 0$) yields $w_m = v/\lambda_m$, whereupon Eq. (168) reduces to:

$$(\tau - \tau_p^{\text{eff}})b = v \sum_{m=1}^2 R_m = B_{\text{drag}} v, \quad (169)$$

confirming consistency with the steady state formulation.

Figure 9 shows the mobility law resulting from the results quoted in Table I for Ni, Cu, Fe, Ta at 300 and 600 K. The model recovers naturally qualitative observations from MD that need not be apparent from perusing the raw drag data in Table I. Indeed, as we have discussed in Sec. IV C, MD data typically report increased apparent drag for screw dislocations over edge dislocations (see, e.g., Ref. [60]), whereas our 0 velocity linear drag coefficients are typically lower for screw dislocations.

This apparent contradiction is resolved by recognizing that MD simulations measure an effective drag averaged over the acceleration transient. As Fig. 9 clearly demonstrates, screw dislocations exhibit dramatically longer acceleration times than edges, reaching steady state only after 0.3–0.4 ps compared to 0.05–0.1 ps for edges. During this extended transient, the dislocation experiences enhanced drag from the slow phonon mode (characterized by λ_2^{-1} in our two-pole model), which dominates the time-integrated response.

The effective drag measured in MD can be approximated as

$$B_{\text{eff}}^{\text{MD}} \approx \frac{1}{t_{\text{sim}}} \int_0^{t_{\text{sim}}} B(t) dt = B_{\infty} + \sum_i \frac{B_i \lambda_i}{t_{\text{sim}}} (1 - e^{-\lambda_i t_{\text{sim}}}). \quad (170)$$

For typical MD simulation times comparable to the slow relaxation time λ_2^{-1} , this integral is dominated by the transient contribution B_2 , which is substantially larger for screws than

edges (see Table I). Only in the long-time limit $t_{\text{sim}} \gg \lambda_2^{-1}$ does the steady state ordering $B_{\infty}^{\text{edge}} > B_{\infty}^{\text{screw}}$ emerge.

This effect is particularly pronounced in Ta, where the screw dislocation shows an exceptionally long transient approaching 0.5 ps at 300 K, consistent with its large B_2/B_{∞} ratio. The temperature dependence further supports this interpretation: at 600 K, the acceleration times decrease for all systems as thermal activation assists in overcoming the transient phonon coupling. Thus what MD interprets as larger drag for screws is actually the signature of their longer-lived phonon memory, captured naturally by our multitimescale kernel formalism.

C. First-principles parameter determination

All parameters in the mobility laws derive systematically from the microscopic theory without empirical fitting. The extraction procedure comprises four stages.

Effective Peierls stress. The temperature-dependent Peierls barrier incorporates both zero-point quantum corrections and thermal lattice expansion through the self-consistent phonon approximation (Sec. V). Starting from the bare Peierls stress $\tau_p^{(0)}$ at $T = 0$, anharmonic renormalization yields

$$\tau_p^{\text{eff}}(T) = \tau_p^{(0)} - \frac{2\pi^2}{b^2} \sum_{\lambda \in \mathcal{C}} \left[\frac{\hbar}{2} (\tilde{\omega}_{\lambda} - \omega_{\lambda}) + k_B T \ln \left(\frac{1 - e^{-\hbar \tilde{\omega}_{\lambda}/k_B T}}{1 - e^{-\hbar \omega_{\lambda}/k_B T}} \right) \right],$$

where the sum extends over phonon modes within the dislocation core region $\mathcal{C}$, and $\tilde{\omega}_{\lambda}(T)$ are the self-consistently renormalized frequencies.

Radiative drag coefficient. From the zero-temperature analysis of Section III, the radiative coefficient follows directly from lattice parameters:

$$C_{\text{rad}}^{(0)} = \frac{\mu b^2}{24\pi \rho c_T^2} \mathcal{A} \int_{k_{\min}}^{k_D} \frac{dk}{k^3}, \quad (171)$$

where the integral is regularized by the infrared cutoff $k_{\min} = 2\pi/L$ (system size) and ultraviolet cutoff $k_D = \pi/a$ (Brillouin zone boundary). For practical calculations with $L \gg a$:

$$C_{\text{rad}}^{(0)} \approx \frac{\mu b^2}{48\pi \rho c_T^2} \mathcal{A} \ln(L/a). \quad (172)$$

Temperature dependence enters through the thermal enhancement factor $(1 + 2k_B T/\hbar \omega_D)$ as established in Eq. (65).

Memory kernel poles. The pole-residue pairs (λ_m, R_m) are extracted through Padé approximation of the computed kernel $\hat{\Gamma}_T(s)$. Following the procedure detailed in Sec. IV C, we

- (1) compute $\hat{\Gamma}_T(s_n)$ on a Tchebycheff grid $s_n \in [10^{-3}, 10^2]$ rad/ps using Eq. (69);
- (2) apply Padé(2, 2) fitting to ensure positivity: $\ln \hat{\Gamma}_T(s) \approx P_2(s)/Q_2(s)$;
- (3) extract poles as roots of $Q_2(s) = 0$ and residues from partial fraction decomposition.

Table I provides a collection of values for λ_m and R_m in a number of fcc and bcc metals.

Temperature scaling. All transport coefficients inherit temperature dependence through the quantum statistical

factor:

$$R_m(T) = R_m^{(0)} \frac{\langle 2n_B(\omega) + 1 \rangle_T}{\langle 2n_B(\omega) + 1 \rangle_0}, \quad (173)$$

where the thermal average extends over the phonon modes contributing to each pole. In the high-temperature limit, this reduces to linear scaling: $R_m(T) \approx R_m^{(0)}(1 + 2k_B T / \hbar \omega_m)$.

D. Bulk viscosity and the line-drag coefficient

Large-scale molecular-dynamics studies often quote a *bulk* phonon-drag (viscosity) in units of Pa s, $\eta(T) \approx 7.5 \times 10^{-8} T$ Pa s, deduced from the average crystal-wide viscous stress $\sigma_{r\theta} = 2\eta \dot{\epsilon}_{r\theta}$ generated by a moving dislocation. Our mobility equations, e.g., Eq. (162), require a *line* drag B in N s m⁻¹: $(\tau - \tau_P^{\text{eff}})b = Bv + C_{\text{rad}}v^4$. At first sight, the units mismatch, but the Keldysh formulation shows that the two quantities differ only by the universal logarithm familiar from continuum dislocation theory.

Indeed, the zero-frequency limit of the Laplace kernel (Sec. IV C) is

$$B_{\text{drag}} = \frac{\hbar}{\rho} \int \frac{d^3k}{(2\pi)^3} \frac{|\Phi_{ij}(\mathbf{k}) B_j|^2}{\omega^3(\mathbf{k})}, \quad (174)$$

where $|\Phi B|^2 / \omega^3 \propto k^{-2}$ for acoustic modes. Splitting $\int d^3k = \int_{k_{\min}}^{k_D} dk 4\pi k^2$ gives the long-wavelength integral

$$B_{\text{drag}} = \underbrace{\frac{\hbar b^2}{2\pi \rho c_T^2}}_{\equiv \eta(T)} 2\pi \ln\left(\frac{k_D}{k_{\min}}\right),$$

which we have rewritten by recognizing the bracketed prefactor as the *bulk* shear viscosity $\eta(T) = \hbar \langle n_B + \frac{1}{2} \rangle / \rho c_T^2$ obtained in MD. Transforming back to real space with $k_{\min} = 2\pi/R$ and $k_D = \pi/a$ therefore yields exactly

$$B = 2\pi \eta(T) \ln(R/r_c), \quad (175)$$

where $r_c \simeq 2b$ is the core radius introduced in the Kanzaki force and R is the outer cutoff (half the MD cell length or the mean dislocation spacing).

Because Eq. (175) follows directly from the kernel integral, the fundamental power balance used throughout the paper, $(\tau - \tau_P^{\text{eff}})bv = P/L = Bv^2$, remains intact. The MD practitioner needs only to multiply the reported $\eta(T)$ by the logarithmic factor $\ln(R/r_c)$ to obtain a line drag consistent with the first-principles mobility laws of Secs. III–VIII.

With that in place, it is possible to further compare our Keldysh results shown in Table I to available experimental data. For Ni, experimental data [139] at room temperature quotes a drag coefficient of $\sim 10^4$ Pa s (similar range is provided by [60] in MD simulations); our own, once converted to bulk data, is 2.56×10^{-4} Pa s. For Fe, Turner, and Vreeland [140] quote drag values that when linearized at room temperature render $\sim 10^{-3}$ Pa s, as opposed to our own of 8.55×10^{-3} Pa s. MD simulations [59] report 2.01×10^{-4} Pa s. For Ta, Baker and Carpenter [141] provide, via the linearized Gilman model, a value of order (without edge/screw distinction) 10^{-4} – 10^{-3} Pa s; our own results range 10^{-3} – 10^{-4} Pa s. As we have already explained in Sec. IV C, care should be taken when comparing Keldysh drags to bulk drags, as the

former are inherently time-dependent; aside from methodological differences in the bulk vs line drag definitions, MD simulations will account for a realistic core structure and typically need to introduce a dissipative layer about the top and bottom surfaces of the crystallite (cf. Ref. [61]).

E. Numerical implementation

The choice between steady state and transient formulations depends on the characteristic loading rate. We define the dimensionless Deborah number [142]:

$$\text{De} = \frac{|\dot{\tau}|}{\tau \lambda_1}, \quad (176)$$

which compares the loading time scale to the fastest phonon relaxation. For $\text{De} < 0.1$, a steady state approximation suffices; otherwise, the full differential system is required.

The implementation algorithm proceeds as follows.

(1) Initialization. Load temperature-dependent parameters $\{\tau_P^{\text{eff}}(T), C_{\text{rad}}(T), \lambda_m(T), R_m(T)\}$ from precomputed tables or analytical fits.

(2) Regime selection. Compute De from the stress history. If $\text{De} < 0.1$, use Eq. (163) directly. Otherwise, proceed to step 3.

(3) Time integration. For the differential system (167) and (168), employ the analytical solution:

$$w_m^{n+1} = w_m^n e^{-\lambda_m \Delta t} + \frac{v^n}{\lambda_m} (1 - e^{-\lambda_m \Delta t}), \quad (177)$$

where superscripts denote time levels.

(4) Velocity solution. Substitute updated w_m^{n+1} into Eq. (168) to obtain:

$$v^{n+1} = \frac{(\tau^{n+1} - \tau_P^{\text{eff}})b}{\sum_{m=1}^2 R_m \lambda_m w_m^{n+1}}. \quad (178)$$

(5) Stability check. Ensure $\Delta t < 0.5 / \max(\lambda_1, \lambda_2)$ for numerical stability. For typical values, this requires $\Delta t < 0.02$ ps.

The steady state law (163) requires only four arithmetic operations per evaluation. The transient model adds two exponential evaluations per time step, negligible compared to typical CPFE stress updates.

F. Application to specific deformation regimes

The unified formulation naturally captures distinct plastic flow regimes through the interplay of stress, temperature, and time scales:

(1) Thermally activated creep ($\tau \lesssim 2\tau_P^{\text{eff}}$). The mobility reduces to $v \approx (\tau - \tau_P^{\text{eff}})b/B_{\text{drag}}$, with activation energy $Q = \tau_P^{\text{eff}}(T)b^3$ governing the temperature sensitivity. This regime dominates at low homologous temperatures and modest stresses.

(2) Phonondrag regime ($2\tau_P^{\text{eff}} < \tau < 100\tau_P^{\text{eff}}$). Both viscous and radiative terms contribute, yielding effective power-law behavior $v \propto \tau^n$ with $1/2 < n < 1$. The exponent varies smoothly with stress, capturing the transition observed in shock experiments.

(3) Radiation-dominated flow ($\tau > 100\tau_P^{\text{eff}}$). The square-root scaling $v \propto \sqrt{\tau}$ emerges from the quadratic drag law

$\tau \propto v^2$, limited ultimately by the transonic resonance analysed in Sec. VI. For fcc metals, this regime typically requires stresses exceeding about 1 GPa (see, e.g., Ref. [60]).

(4) Dynamic overshoot. Under rapid loading ($De > 1$), the transient formulation predicts velocity overshoot followed by exponential relaxation to steady state. The overshoot magnitude scales as $(1 - e^{-\lambda_1 t_{\text{rise}}})$ where t_{rise} is the stress rise time.

The framework extends systematically to more complex scenarios. For instance, in nonisothermal conditions, temperature variations enter through the explicit T dependence of all parameters. For heating rates $\dot{T} < 10^6$ K/s, quasistatic parameter updates suffice. Rapid thermal transients require coupling to the heat equation through the dissipated power P_{diss} . Multiaxial stress states are easily dealt with: for nonglide stresses, project onto the slip system: $\tau = \boldsymbol{\sigma} : (\mathbf{s} \otimes \mathbf{n})$, where $\mathbf{s}$ and $\mathbf{n}$ are slip direction and normal. Cross-slip activation requires a separate mobility evaluation for each viable system. The crystal structures used here (fcc) are just an example taken to showcase the methodology, which is entirely universal and applicable to any alternative crystal structures. One must be careful when computing geometric factor $\mathcal{A}$ and cutoff structures, as these do vary with crystal symmetry. For hcp metals, for instance, one can distinguish basal ($\mathcal{A} = 0.82$) from prismatic ($\mathcal{A} = 0.94$) slip. Finally, our treatment is readily extensible to mixed character dislocations: for relatively low curvature lines in cubic and hcp crystals, the radiative drag reduces to the simple interpolation $B(\chi) = B_{\text{screw}} \cos^2 \chi + B_{\text{edge}} \sin^2 \chi$ for $\chi = \arccos(\mathbf{b} \cdot \mathbf{t}/|\mathbf{b}|)$ the character angle, with the derivation and limits of validity discussed in Appendix G.

Nevertheless, our systematic reduction from first-principles theory to implementable mobility laws enables predictive plasticity modeling across all relevant deformation regimes without empirical parameters, and without the need for computationally costly parametrizations using MD. We must emphasize here that our mobility framework includes from first principles all atomistic effects that can *in principle* be obtained from MD simulations, so long as the dislocation has achieved a state of glide. Although core effects and Peierls barriers are included, our formulation does not account for activation of motion effects, which require a distinct treatment focused on the stochastics of Peierls barrier hopping by dislocation kinks, as may be found in, e.g., Ref. [24].

IX. CONCLUSIONS

We have developed a comprehensive quantum statistical theory of dislocation mobility that provides a unified treatment across all velocity regimes from first principles. The formulation rests on three key innovations: (i) the use of discrete Kanzaki forces to capture the topological nature of dislocations while maintaining exact force balance, (ii) the application of Keldysh nonequilibrium field theory to properly account for quantum statistics and thermal effects, and (iii) the inclusion of anharmonic corrections through a conserving Baym-Kadanoff approach that preserves fundamental conservation laws. Together, these elements yield a parameter-free theory once harmonic and anharmonic force constants are specified.

The central result of this work is the derivation of a universal memory kernel $\Gamma_T(\theta)$ that encodes all phononmediated dissipation mechanisms within a single, calculable function. At zero temperature, this kernel reduces to the exact result for spontaneous phonon emission, yielding the classical [21] drag law $\tau \propto v^2$ with no adjustable parameters. The discrete lattice structure provides natural regularization, eliminating the divergences at sound speeds that have plagued continuum theories since Eshelby's foundational work [17–19]. At finite temperature, our Keldysh formalism automatically incorporates both stimulated emission and absorption processes, reproducing the experimentally observed linear temperature dependence of phonon drag while maintaining the correct quantum-to-classical crossover. At the same time, it offers a physically insightful way of modeling dislocation drag, not as a result of a fit to observables, but rather as a reactive process that measures the energy dissipated over time through active phonon channels.

This memory kernel $\Gamma_T(t)$ shows that dislocation drag is not instantaneous: it encapsulates an acoustic relaxation (~ 0.01 ps), followed by a slower longitudinal mode response (~ 1 ps). Dislocations then remember their past motion through lingering phonon excitations, which explains why MD simulations see different drag for edges vs screws: they are measuring different parts of the transient response, which our formalism can now qualify and quantify to show that drag emerges from the quantum field theory of dislocation-phonon interaction.

The inclusion of anharmonic effects through self-consistent phonon theory represents a significant advance over existing treatments. Finite phonon lifetimes emerge naturally from three-phonon processes, converting mathematical singularities into physical resonances of finite width. The temperature-dependent frequency renormalization reduces effective Peierls barriers, while the imaginary parts of the self-energies provide intrinsic broadening that eliminates the need for phenomenological damping parameters. Crucially, this anharmonic treatment preserves the gauge invariance and conservation laws of the underlying lattice theory.

Our systematic reduction from the full quantum field theory to practical mobility laws addresses a longstanding challenge in multiscale modeling. Through controlled approximations, each with explicit error bounds, we derive both steady state and transient formulations suitable for implementation in engineering codes. The steady state law interpolates smoothly between viscous drag at low velocities and radiation-dominated behavior near sound speeds. The transient formulation, expressed as a minimal set of auxiliary differential equations, captures memory effects essential for shock and high-rate loading while adding negligible computational cost.

In practical terms, the formulation bridges disparate physical regimes within a single, consistent framework. From quasistatic creep through viscous drag to radiation-limited motion, each regime emerges naturally without regime-specific modifications or matching conditions. The mobility law transitions continuously from $\tau \propto Tv$ at low velocities to enhanced but finite drag near sound speeds, with the crossover points determined entirely by material constants. This unified treatment eliminates the need for piecewise mobility

models that have historically required empirical fitting at regime boundaries. Moreover, the theory's expression solely in terms of force constants means that mobility laws for new materials or extreme conditions can be predicted *ab initio*, transforming dislocation dynamics and crystal plasticity simulations from interpolative to genuinely predictive tools. The resulting closure relation offers direct access to strain rate sensitivity, thermal hardening, and transonic phenomena, all traceable to the same microscopic physics without phenomenological intervention, or without the need to perform costly campaigns of molecular dynamics simulations of dislocation mobility [143].

Several specific predictions emerge that are amenable to experimental verification. First, the theory predicts a universal scaling of the drag coefficient with $(1 + 2k_B T / \hbar \omega_D)$ that should hold across all materials once geometric factors are accounted for. Second, the transition from viscous to radiative drag should occur at a critical velocity determinable from elastic constants alone, providing a stringent test requiring no adjustable parameters. Third, the predicted enhancement of drag near sound speeds, finite but substantial, should be observable in shock experiments approaching the transonic regime. Recent advances in ultrafast electron microscopy may soon enable direct validation of these predictions.

Five avenues appear most compelling for future work. First, coupling the present phononic sector to electron Green functions would expose the relative weight of electron scattering and magnetoplastic effects, thereby extending predictive reach to low temperatures and high magnetic fields. Second, the analytic structure of the self-energies suggests that mass-disorder scattering and solute drag may enter as straightforward generalizations once the alloy dynamical matrix is available, opening the door to truly multicomponent mobility laws. Third, the relative role of the core structure in anharmonic radiation warrants further investigation, particularly in systems most likely to display strong anharmonicities, as may be high entropy alloys. Fourth, the role of the kink-pair mechanism in the activation of the motion regime has been simplified to a hopping rate; further work ought to couple the present formalism to the Frenkel-Kontorova style stochastic frameworks employed in their modeling, as well as to the role of line curvature and mixed character behavior in drag. Finally, embedding the theory in large scale dislocation-dynamics [4,143] and CPFE codes [144] will permit systematic interrogation of strain-rate effects in shock, ramp and cyclic loading and, by confronting simulation with emerging ultrafast characterization data, will close the remaining loop between first-principles kinetics and macroscopic constitutive response.

In summary, this work establishes a rigorous theoretical foundation for understanding dislocation mobility across all physically relevant regimes. By demonstrating that phonon-mediated drag can be calculated exactly from lattice dynamics, without empirical parameters or artificial regularization, we provide both fundamental insight and practical tools for predictive materials modeling. The framework's ability to bridge quantum mechanics and continuum plasticity through systematic, controlled approximations represents a step up toward truly multiscale constitutive laws grounded in atomic-level physics.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [145].

APPENDIX A: CORE MULTIPOLES IN THE HARMONIC LATTICE

This Appendix formalizes the core contribution as a discrete multipolar expansion and clarifies how the effective dipole representation used in the main text arises from a systematic Taylor expansion of the lattice response. The lattice Kanzaki representation splits the total dislocation force into a slip term, derived from the Volterra affine mapping, and a core term, representing discrete residuals localized in the atomic core. While the slip contribution governs infrared (long-wavelength) behavior and recovers classical elasticity in the continuum limit, the core term dominates ultraviolet physics and introduces higher-gradient corrections, necessary for properly regularising lattice radiation and mobility in the quantum-thermal regime.

Discrete core force definition. The core force density in real space is represented as a sum of localized atomic point forces moving at the dislocation glide speed v_d :

$$f_i^{\text{core}}(\mathbf{r}, t) = \sum_n f_i^n \delta^{(3)}(\mathbf{r} - \mathbf{R}_n - v_d t \hat{\mathbf{e}}_{\parallel}), \quad \mathbf{R}_n \in \text{core}, \quad (\text{A1})$$

where f_i^n is the microscopic force applied to the n th core atom, $\mathbf{R}_n$ its equilibrium lattice position, and $\hat{\mathbf{e}}_{\parallel}$ the unit vector along the glide direction. This form ensures Galilean invariance by encoding the rigid translation of the dislocation core. The force density $f_i^{\text{core}}(\mathbf{r}, t)$ has units of force per unit volume.

The harmonic displacement response is given by convolution with the causal Green operator:

$$u_i(\mathbf{r}, t) = \sum_n \int_{-\infty}^t dt' G_{ij}(\mathbf{r} - \mathbf{R}_n - v_d t' \hat{\mathbf{e}}_{\parallel}, t - t') f_j^n. \quad (\text{A2})$$

The Green function $G_{ij}(\mathbf{r}, t)$ solves the lattice wave equation with force-constant kernel $\Phi_{ij}(\mathbf{r} - \mathbf{r}')$, satisfies causality, and is translationally invariant.

The Fourier transform of the core force density (A1) reads

$$\tilde{f}_i^{\text{core}}(\mathbf{k}, \omega) = \sum_n f_i^n e^{-i\mathbf{k} \cdot \mathbf{R}_n} \int dt e^{i\omega t} \delta(t - (x_{\parallel} - R_{\parallel,n})/v_d) \quad (\text{A3})$$

$$= 2\pi \sum_n f_i^n e^{-i\mathbf{k} \cdot \mathbf{R}_n} \delta(\omega - v_d k_{\parallel}), \quad (\text{A4})$$

where $k_{\parallel} = \mathbf{k} \cdot \hat{\mathbf{e}}_{\parallel}$ and $R_{\parallel,n} = \mathbf{R}_n \cdot \hat{\mathbf{e}}_{\parallel}$. This confirms that the core force spectrum shares the same Doppler constraint

$\omega = v_d k_{\parallel}$ as the slip contribution. The spatial kernel may now be expanded in a Taylor series about the dislocation line.

Imposing the equilibrium constraints

$$\sum_n f_i^n = 0, \quad \sum_n (f_i^n R_n^j - f_j^n R_n^i) = 0, \quad (\text{A5})$$

ensures no monopole or net torque arises. The leading nonvanishing moment is then the symmetric force dipole:

$$M_{ij}^{(1)} = \sum_n f_i^n R_n^j. \quad (\text{A6})$$

Expanding the exponential $e^{-i\mathbf{k}\cdot\mathbf{R}_n}$ to first order gives

$$\sum_n f_i^n e^{-i\mathbf{k}\cdot\mathbf{R}_n} = -ik_j M_{ij}^{(1)} + \frac{1}{2} k_j k_k M_{ijk}^{(2)} + \dots, \quad (\text{A7})$$

where $M_{ijk}^{(2)} = \sum_n f_i^n R_n^j R_n^k$ is the quadrupole moment. Higher order multipole moments would be taken similarly. Thus, the Fourier-transformed core force reads

$$\tilde{f}_i^{\text{core}}(\mathbf{k}, \omega) = -ik_j M_{ij}^{(1)} (2\pi) \delta(\omega - v_d k_{\parallel}) + \dots \quad (\text{A8})$$

in the long-wavelength limit. This explicitly identifies the effective dipole moment $M_{ij}^{(1)}$ that enters the low- k lattice radiation and mobility laws.

Inverting the Fourier transform to leading order yields

$$f_i^{\text{core}}(\mathbf{r}, t) = \partial_j [M_{ij}^{(1)} \delta(\mathbf{r} - v_d t \hat{\mathbf{e}}_{\parallel})] + \mathcal{O}(\nabla^2). \quad (\text{A9})$$

This form recovers the dipole representation used in the main text. The force density is localized on the instantaneous dislocation position and applies a pair of opposite forces separated across the core width. Its divergence-free character follows from the symmetry and equilibrium constraints above.

In the long-wavelength regime $k \ll a^{-1}$, the slip term dominates and generates classical fields [86]. The core contribution enters through the dipole $M_{ij}^{(1)}$ and becomes relevant for $k \gtrsim 1/R_{\text{core}}$. In practice, the magnitude of $M_{ij}^{(1)}$ is of order $\mu b^2 R_{\text{core}}$ and its radiated power contribution scales as k^2 relative to the leading slip. Thus, for typical dislocation cores $R_{\text{core}} \sim 2b$ and speeds below $0.8c_T$, core-induced corrections to radiation remain below the percent level.

For a typical edge dislocation, the dipole tensor has magnitude $|M^{(1)}_{ij}| \sim \mu b^2 R_{\text{core}}$ with $R_{\text{core}} \sim 2b$, consistent with *ab initio* estimates for Al and Ni. This gives $M^{(1)} \sim 10^{-19}$ N m, leading to $<1\%$ contribution to radiative drag below $0.8c_T$.

The symmetry of $M_{ij}^{(1)}$ reflects the character of the dislocation: edge dipoles respect mirror symmetry and have even parity across the slip plane, while screw dipoles generate antisymmetric force fields. Higher-order moments such as $M_{ijk}^{(2)}$ contribute at order k^3 and are negligible for mobility up to intermediate velocities.

In practice, the dipole moment $M^{(1)}_{ij}$ may be extracted from MD or *ab initio* calculations by extracting the Kanzaki forces and performing the multipolar expansion [74].

APPENDIX B: FOURIER-LAPLACE TRANSFORM

Define

$$\tilde{F}_i(\mathbf{k}, \omega) = \sum_{\mathbf{r}} \int_{-\infty}^{\infty} dt e^{i(\omega t - \mathbf{k}\cdot\mathbf{r})} F_i^{\text{slip}}(\mathbf{r}, t),$$

and insert the real-space force. Translational invariance of Φ_{ij} gives

$$\sum_{\mathbf{r}} e^{-i\mathbf{k}\cdot\mathbf{r}} \Phi_{ij}(\mathbf{r} - \mathbf{r}') = \Phi_{ij}(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{r}'}.$$

Hence

$$\tilde{F}_i(\mathbf{k}, \omega) = -\Phi_{ij}(\mathbf{k}) B_j \sum_{\mathbf{r}'} e^{-i\mathbf{k}\cdot\mathbf{r}'} \Psi(\mathbf{r}') I(\omega; x'_{\parallel}),$$

with

$$I(\omega; x'_{\parallel}) = \int_{-\infty}^{\infty} dt e^{i\omega t} \Theta(x'_{\parallel} - v_d t).$$

Assume $v_d > 0$ (the opposite sign is obtained by analytic continuation):

$$\Theta(x'_{\parallel} - v_d t) = \Theta(t_0 - t), \quad t_0 = x'_{\parallel}/v_d.$$

Using the distribution identity $\int_{-\infty}^a e^{i\omega t} dt = \pi \delta(\omega) + e^{i\omega a}/(i\omega)$ gives

$$I(\omega; x'_{\parallel}) = \pi \delta(\omega) + \frac{e^{i\omega x'_{\parallel}/v_d}}{i\omega}.$$

The first term ($\propto \delta(\omega)$) generates only a static $\omega = 0$ contribution and plays no role in radiation, so we keep the second term.

Insert $I(\omega; x'_{\parallel})$ and separate the $x'_{\parallel}$ -dependent phase:

$$e^{-i\mathbf{k}_{\parallel} x'_{\parallel}} e^{i\omega x'_{\parallel}/v_d} = e^{-ix'_{\parallel}(k_{\parallel} - \omega/v_d)}.$$

Hence

$$\sum_{\mathbf{r}'} e^{-i\mathbf{k}_{\perp}\cdot\mathbf{r}'_{\perp}} \Psi(\mathbf{r}') e^{-ix'_{\parallel}(k_{\parallel} - \omega/v_d)} = \tilde{\Psi}(\mathbf{k}) (2\pi) \delta(k_{\parallel} - \omega/v_d),$$

because $\Psi(\mathbf{r}')$ is nonzero only on bonds crossing the glide plane and its Fourier transform is $\tilde{\Psi}(\mathbf{k}) \propto \delta(k_{\perp}) \delta(k_3) \text{sgn } k_{\parallel}$.

Collecting factors,

$$\tilde{F}_i(\mathbf{k}, \omega) = -\Phi_{ij}(\mathbf{k}) B_j \tilde{\Psi}(\mathbf{k}) \frac{(2\pi) \delta(k_{\parallel} - \omega/v_d)}{i\omega}.$$

Replace the δ -function argument: $\delta(k_{\parallel} - \omega/v_d) = (v_d)^{-1} \delta(\omega - v_d k_{\parallel})$. Finally write $1/(i\omega) = 1/[iv_d k_{\parallel}] = -1/(k_{\parallel} + i0^+)$, where the $i0^+$ ensures the correct causal prescription inherited from the Laplace transform of the Heaviside step. Thus

$$\tilde{F}_i(\mathbf{k}, \omega) = -\frac{\Phi_{ij}(\mathbf{k}) B_j \tilde{\Psi}(\mathbf{k})}{k_{\parallel} + i0^+} (2\pi) \delta(\omega - v_d k_{\parallel}),$$

which is Eq. (24). The derivation shows that the $(k_{\parallel} + i0^+)^{-1}$ factor comes directly from the Laplace–Fourier transform of the sliding Heaviside cut, while the Doppler delta $\delta(\omega - v_d k_{\parallel})$ follows from phase matching along the glide axis.

APPENDIX C: PRACTICAL NUMERICAL REALIZATION OF THE KERNEL OF EQ. (67)

The computation starts from a harmonic force model that supplies the dynamical matrix $D_{i\ell}(\mathbf{k})$ of the crystal. Any source is admissible: density-functional perturbation theory, a classical second-moment potential, or a tabulated Born-von Kármán fit. What matters is that for every wave vector on the

longitudinal line $k_{\parallel} \hat{\mathbf{x}}$ it yields the eigenfrequencies $\omega_{\alpha}(k_{\parallel})$ and the (mass-weighted) polarization vectors $\tilde{e}_i^{(\alpha)}(k_{\parallel})$.

Slip-coupling amplitude. The discrete Kanzaki force $\Phi_{ij}B_j$ is evaluated in reciprocal space either by finite differences of the force constants or, when a continuous potential is at hand, by analytic differentiation. The mass weighting used by most phonon codes is removed by multiplying the polarization vector by $\sqrt{m_i}$. The contraction $C_{\alpha}(k_{\parallel}) = \tilde{e}_i^{(\alpha)}\Phi_{ij}B_j$ is produced in units of $\text{eV } \text{\AA}^{-1}$.

One-dimensional mesh. The three-dimensional Brillouin integral collapses to a single line integral over $k_{\parallel}$ because the two transverse Dirac deltas pin $k_{\perp} = k_3 = 0$. A linear mesh $k_{\parallel,n} = k_{\min} + n\Delta k$ with $k_{\min} = 2\pi/L$ covers the domain $k_{\min} \leq k_{\parallel} \leq k_D$, where $k_D = \pi/a$ is the Debye cutoff of a monatomic cubic lattice. Nyquist theory [146] shows that for a time window $0 \leq \theta \leq \theta_{\max}$ the spacing must satisfy $v_s \Delta k \ll \pi/\theta_{\max}$ with v_s the largest acoustic velocity. For aluminium, $v_s \simeq 6 \times 10^3 \text{ m s}^{-1}$ and $\theta_{\max} = 0.5 \text{ ps}$ require $\Delta k \lesssim 10^{-4} \text{ \AA}^{-1}$, about eight thousand nodes on a linear grid. A geometric mesh $k_{\parallel,n} = k_{\min}(k_D/k_{\min})^{n/(N_k-1)}$ achieves the same resolution with one tenth as many points because the integrand scales as $|k_{\parallel}|^{-1}$ and is therefore dominated by the long-wavelength region.

Discrete kernel. The memory kernel per unit dislocation length is obtained from

$$\Gamma_T(\theta) = \frac{\hbar b^2}{\rho} \sum_{\alpha,n} \frac{|C_{\alpha}(k_{\parallel,n})|^2}{\omega_{\alpha}(k_{\parallel,n}) |k_{\parallel,n}|} [2n_B(\omega_{\alpha}) + 1] \times \cos[\omega_{\alpha}(k_{\parallel,n})\theta] \Delta k, \quad (\text{C1})$$

where $b = |\mathbf{b}|$ and ρ is the three-dimensional mass density. No cross-sectional area appears because the two collapsed Dirac deltas have already supplied the length scale.

Avoiding aliasing. Equation (C1) is accurate only for $\theta < \pi/(v_s \Delta k)$. Beyond that time the oscillatory cosine is under-resolved and neighboring terms fail to cancel, producing the artificial shoulder visible in a coarse grid. Two

remedies are available. Either increase N_k until the Nyquist condition holds for the desired $\theta_{\max}$ or replace the direct time-domain evaluation by a Laplace-space procedure: $\hat{\Gamma}_T(s) = \sum_{\alpha,n} |C_{\alpha}|^2 [2n_B + 1]/(k_{\parallel,n}(\omega_{\alpha}^2 + s^2)) \Delta k$ for real positive s , fit $\ln \hat{\Gamma}_T(s)$ with an (M, M) Padé approximant, exponentiate, and invert analytically. For aluminium, two poles suffice; the result reproduces the direct sum within one part in 10^3 and is alias-free for every $\theta > 0$.

Here, we used a 48001-point linear grid, a classical second-nearest fcc force model refitted to the experimental Debye temperature, and the Padé reconstruction with $M = 2$ give $\Gamma_T(0) = 4.6 \times 10^{-5} \text{ N}$ at $T = 300 \text{ K}$ and $1.6 \times 10^{-4} \text{ N}$ at $T = 600 \text{ K}$, consistent with phonondrag data obtained from MD simulations [60]. The code used to generate Fig. 2 relies only on NUMPY for array algebra and SCIPY for the Padé fit, and runs in under five minutes on a laptop. Any language that supports eigendecomposition, elementary quadrature and a nonlinear least-squares routine can be employed. The phonon modes were calculated using Phonopy [147] and Phonolammps [104] via Lammps [148]. Geometrical input files were generated using Atomsk [149].

APPENDIX D: SOLUTION PROCEDURE FOR THE LOCAL ODE SYSTEM OF THE NON-LINEAR QUANTUM THERMAL MOBILITY LAW

The coupled equations form a linear, time-invariant system once the velocity excursion $\delta v(t) = v(t) - v_0$ is treated as the state variable and each auxiliary amplitude $w_m^{(n)}$ is appended. Collecting the unknowns in the column vector

$$\mathbf{y}(t) = (v(t), w_1^{(0)}, w_2^{(0)}, w_1^{(1)}, w_1^{(2)}, w_1^{(3)})^T,$$

the hierarchy may be written compactly as

$$\dot{\mathbf{y}}(t) = \mathbf{A} \mathbf{y}(t) + \mathbf{f},$$

where $\mathbf{f} = (\tau b / \sum_n B_T^{(n)}, 0, \dots, 0)^T$ is the constant drive and $\mathbf{A}$ is the upper diagonal matrix

$$\mathbf{A} = \begin{pmatrix} -\frac{(\sum_n B_T^{(n)})^2}{\tau b \sum_n B_1^{(n)}} & -\tau b R_1^{(0)} & -\tau b R_2^{(0)} & -\tau b R_1^{(1)} & -\tau b R_1^{(2)} & -\tau b R_1^{(3)} \\ 0 & -\lambda_1^{(0)} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\lambda_2^{(0)} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\lambda_1^{(1)} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\lambda_1^{(2)} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\lambda_1^{(3)} \end{pmatrix}.$$

Because $\mathbf{A}$ possesses real, strictly negative eigenvalues $-\lambda_m^{(n)}$ together with one additional negative root supplied by the prefactor in the first row, the system is Lyapunov stable and diagonalizes without Jordan blocks. The formal solution is therefore [150]

$$\mathbf{y}(t) = e^{\mathbf{A}t} \mathbf{y}(0) + (\mathbf{1} - e^{\mathbf{A}t}) \mathbf{A}^{-1} \mathbf{f}.$$

For the truncated aluminium hierarchy $(N, M) = (3, 1)$ the matrix is only 6×6 ; its exponential can be evaluated analytically as a sum of six simple exponentials or, more

conveniently, by a single call to a stable Padé-scaled squaring algorithm.

For the one-pole nonlinear truncation $(N, M) = (3, 1)$ with vanishing initial auxiliary variables $w_1^{(n)}(0) = w_2^{(0)}(0) = 0$ the six-dimensional system is diagonal in Laplace space and can be solved in closed form. Introduce the shorthand

$$K \equiv \frac{(\sum_{n=0}^3 B_T^{(n)})^2}{\tau b \sum_{n=0}^3 B_1^{(n)}}, \quad v_{\infty} \equiv \frac{\tau b}{\sum_n B_T^{(n)}},$$

and denote the pole set $\{\lambda_1^{(0)}, \lambda_2^{(0)}, \lambda_1^{(1)}, \lambda_1^{(2)}, \lambda_1^{(3)}\}$ collectively by λ_j with residues $\mathcal{R}_j \in \{R_1^{(0)}, R_2^{(0)}, R_1^{(1)}, R_1^{(2)}, R_1^{(3)}\}$. Solving the auxiliary equations first and inserting them into $\dot{v}$ one finds

$$v(t) = v_\infty + (v_0 - v_\infty)e^{-Kt} - \tau b \sum_j \frac{\mathcal{R}_j}{1 - \lambda_j/K} (e^{-\lambda_j t} - e^{-Kt}).$$

The first term is the steady velocity, the second describes exponential relaxation on the acoustic time scale K^{-1} , and the third represents the Debye-limited memory carried by the five auxiliary variables. In aluminium at $T = 300$ K the numerical values $K^{-1} \simeq 0.69$ ps and $\lambda_j^{-1} \in \{0.04, 0.7, 0.04, 0.014, 0.010\}$ ps yield a double-exponential transient that is already within 1% of v_∞ after 1 ps and entirely governed by the linear kernel beyond that time.

Otherwise, the problem may be solved numerically. Time-stepping codes need not form the exponential explicitly: a fourth-order Runge–Kutta scheme with a 0.01 ps step ought to be enough to converge to machine precision because the fastest pole, $\lambda_1^{(1)} \approx 100$ ps $^{-1}$, still resolves into a dozen sub-steps. Stiff solvers, such as Rosenbrock-W or implicit BDF [151], handle the same system with tenfold larger steps when the motion is driven by mesoscale stresses that vary on picosecond horizons.

Once $v(t)$ is obtained the displacement moments $\Delta X^{(n)}(t)$ follow from single quadratures, closing the loop for the next time step. Because every kernel moment $B_T^{(n)}$ and $B_1^{(n)}$ is temperature dependent only through its amplitude, thermal changes can be accommodated by updating the diagonal entries of $\mathbf{A}$ and the constant vector $\mathbf{f}$ without touching the solver's numerical scaffold.

APPENDIX E: EXTRACTION OF ANHARMONIC LINEWIDTHS AND EVALUATION OF THE DAMPED MEMORY KERNEL

1. Mode-resolved linewidths $\gamma_\alpha(\mathbf{k}, T)$ from molecular-dynamics trajectories

The exponential damping constants that enter the anharmonic kernel are identified with the half width at half maximum (HWHM) of the phonon spectral function. Following Dynaphopy [122] and the autocorrelation method [121], they are obtained in five steps.

(1) *Trajectory generation.* A microcanonical MD trajectory is run in a $5 \times 5 \times 5$ cubic supercell (500 ps total length, time step 0.5 fs) at each temperature of interest. Atomic positions and velocities $\{\mathbf{R}_i(t), \mathbf{v}_i(t)\}$ are stored every 5 steps to suppress I/O overhead while retaining Nyquist coverage of the Debye frequency.

(2) *Projection onto harmonic eigenmodes.* Harmonic frequencies $\omega_\alpha(\mathbf{k})$ and mass-weighted eigenvectors $\tilde{e}_i^{(\alpha)}(\mathbf{k})$ are taken from the PHONOPY dynamical matrix of Sec. IV C. For every commensurate wave vector in the supercell the mode amplitude is

$$P_{\alpha\mathbf{k}}(t) = \frac{1}{\sqrt{N_c}} \sum_i \sqrt{m_i} \tilde{e}_i^{(\alpha)*}(\mathbf{k}) \mathbf{v}_i(t) e^{i\mathbf{k} \cdot \mathbf{R}_i(t)}, \quad (\text{E1})$$

where N_c is the number of primitive cells.

(3) *Velocity autocorrelation and power spectrum.* The mode-resolved autocorrelation $C_{\alpha\mathbf{k}}(t) = \langle P_{\alpha\mathbf{k}}(0) P_{\alpha\mathbf{k}}^*(t) \rangle$ is evaluated by block averaging over the trajectory. Its discrete Fourier transform $S_{\alpha\mathbf{k}}(\omega) = \int_{-\infty}^{\infty} e^{i\omega t} C_{\alpha\mathbf{k}}(t) dt$ exhibits a single peak for each weakly damped mode.

(4) *Lorentzian fit and quantum rescaling.* Under the weak-damping assumption $S_{\alpha\mathbf{k}}$ is fitted with

$$S_{\alpha\mathbf{k}}(\omega) = \frac{k_B T}{\tilde{\omega}_\alpha(\mathbf{k})} \frac{2\gamma_\alpha(\mathbf{k}, T)}{[\omega - \tilde{\omega}_\alpha(\mathbf{k}, T)]^2 + \gamma_\alpha^2(\mathbf{k}, T)}.$$

The center gives the renormalised frequency $\tilde{\omega}_\alpha$, the HWHM yields $\gamma_\alpha = 1/2\tau_\alpha$. To account for quantum statistics the classical linewidth is multiplied by the ratio $\coth[\hbar\tilde{\omega}_\alpha/2k_B T]/(2k_B T/\hbar\tilde{\omega}_\alpha)$.

(5) *Interpolation to the slip line.* The resulting tables $\tilde{\omega}_\alpha(\mathbf{k}, T)$ and $\gamma_\alpha(\mathbf{k}, T)$ are spline interpolated onto the one-dimensional $k_\parallel$ mesh used in the Volterra integral, enforcing the symmetry $\gamma_\alpha(-k_\parallel) = \gamma_\alpha(k_\parallel)$.

In the present work, these steps were automated with the open-source package *DynaPhoPy* [122]. Convergence tests showed that a 500 ps trajectory yields linewidths stable to better than 5%.

2. Evaluation of the damped memory kernel

Replacing $\omega_\alpha \rightarrow \tilde{\omega}_\alpha$ and introducing γ_α in the denominator turns Eq. (69) into the Laplace-space expression

$$\hat{\Gamma}_{\text{anh}}(s) = \frac{\hbar b^2}{\rho} \sum_\alpha \int_{k_{\min}}^{k_D} \frac{dk_\parallel}{\pi} \frac{|C_\alpha(k_\parallel)|^2}{\tilde{\omega}_\alpha(k_\parallel) |k_\parallel|} [2n_B(\tilde{\omega}_\alpha) + 1] \times \frac{s + \gamma_\alpha}{(s + \gamma_\alpha)^2 + \tilde{\omega}_\alpha^2}. \quad (\text{E2})$$

The same logarithmic $k_\parallel$ grid and adaptive Gauss-Legendre quadrature used for the harmonic case yield $\hat{\Gamma}_{\text{anh}}(s)$ on a Tchebycheff mesh of s -points (10^{-3} – 10^2 rad ps $^{-1}$). The zero-frequency drag and inertial moments follow from $B_T = \hat{\Gamma}_{\text{anh}}(0)$, $B_1 = -\partial_s \hat{\Gamma}_{\text{anh}}|_{s=0}$. A Padé (2,2) fit of $\ln \hat{\Gamma}_{\text{anh}}(s)$ reproduces the numeric data to better than 10^{-3} for all temperatures considered, delivering two pairs (R_m, λ_m) whose real parts now include the anharmonic damping. The inverse Laplace transformation gives the auxiliary ODE system quoted in Sec. V, which may then be integrated with any ODE solver.

APPENDIX F: QUANTITATIVE ESTIMATE OF RADIATIVE DRAG ENHANCEMENT NEAR THE SOUND SPEED

In the principal text, the radiative power associated with a gliding dislocation is written

$$P(v_d, T) = \sum_\alpha \sum_{\mathbf{k} \in \text{BZ}} |V_\alpha(\mathbf{k})|^2 [2n_B(\omega_\alpha) + 1] \times \frac{\gamma_\alpha}{(\omega_\alpha - v_d k_\parallel)^2 + \gamma_\alpha^2}.$$

This Appendix recasts the expression into a dimensionless form that isolates the physical cutoff responsible for eliminating the Eshelby sound barrier, and it provides a concise estimate for the resulting amplification of the drag coefficient in realistic crystals.

Dimensionless reduction. Write $x = \omega/\omega_D$ and $q = k/k_D$ with $0 \leq x, q \leq 1$. Near the sound speed the Doppler shell occupies a narrow annulus around $x = v_d q_{\parallel}/c_T$. Linearising the acoustic branch for $q \ll 1$ and adopting a quadratic expansion $\omega(x) = \omega_D[1 - \frac{1}{2}(1 - q)^2]$ for $q \lesssim 1$ gives

$$P(v_d) \simeq \frac{\rho b^2 v_d^3}{8\pi c_T^4} \mathcal{I}(v_d), \quad \mathcal{I}(v_d) = \int_0^{q_{\max}(v_d)} \frac{q^4 dq}{(1 - q)^2 + \tilde{\gamma}^2},$$

where $\tilde{\gamma} = \gamma/\omega_D \simeq 10^{-3}$ to 10^{-2} is the dimensionless anharmonic linewidth and $q_{\max}(v_d) = v_d/c_T$.

Analytical estimate. The integral can be evaluated in closed form; to leading logarithmic accuracy

$$\mathcal{I}(v_d) \approx \frac{1}{2} \left[\ln \left(\frac{1}{\tilde{\gamma}^2} \right) + 1 - \frac{v_d}{c_T} \right].$$

Hence the drag amplification relative to the quasistatic limit $P_0 \equiv P(v_d \ll c_T)$ reads

$$\frac{P(v_d)}{P_0} \approx 1 + \frac{v_d^2}{c_T^2} \left[\ln \left(\frac{1}{\tilde{\gamma}^2} \right) + 1 - \frac{v_d}{c_T} \right].$$

Taking $\tilde{\gamma} = 5 \times 10^{-3}$ (representative of ferritic iron at ambient temperature) yields a bracket of approximately 6.6, whereas $\tilde{\gamma} = 10^{-2}$ (representative of aluminium) gives 4.6. Within the experimentally accessible velocity interval from $0.7c_T$ up to $0.95c_T$, we therefore anticipate an enhancement

$$30 \lesssim P/P_0 \lesssim 120.$$

Practical rule of thumb. The continuum divergence is cut off when the Doppler shell width falls below the anharmonic linewidth, giving

$$\frac{P(v_d)}{P_0} \approx \frac{1}{\sqrt{1 - (v_d/c_T)^2}} \rightarrow \frac{1}{\sqrt{2}\tilde{\gamma}} \quad \text{as } v_d \rightarrow c_T^-.$$

With $\tilde{\gamma}$ between 10^{-3} and 10^{-2} this ceiling lies between thirty and three hundred, in agreement with the atomistic data quoted above. For crystal-plasticity implementations one may therefore cap the radiative drag as

$$B_{rad}(v_d) \equiv \frac{dP}{dv_d} \simeq B_0 \frac{v_d/c_T}{\sqrt{1 - v_d^2/c_T^2}} \Theta(\sqrt{2}\tilde{\gamma} - \sqrt{1 - v_d^2/c_T^2}),$$

with B_0 the low-velocity limit. This prescription removes the fictitious sound barrier yet retains the physically important rise in radiative damping that governs the transition from subsonic to transonic glide.

APPENDIX G: MIXED CHARACTER DISLOCATIONS AND DRAG

Within the discrete Kanzaki force framework used in this work, a dislocation of mixed character is described by a Burgers vector $\mathbf{b}$ and a line direction $\mathbf{t}$ forming a character angle $\chi = \arccos(\mathbf{b} \cdot \mathbf{t}/|\mathbf{b}|)$. For straight dislocations and wavevectors constrained to the transverse plane ($k_3 = 0$), the lattice dynamical matrix is block diagonal with respect to polarizations parallel and perpendicular to $\mathbf{t}$. The Kanzaki force of a pure screw defect, $\mathbf{F}^{sc}(\mathbf{k})$, is parallel to $\mathbf{t}$, whereas the Kanzaki force of a pure edge defect, $\mathbf{F}^{ed}(\mathbf{k})$, lies in the glide plane and is orthogonal to $\mathbf{t}$. A mixed dislocation can therefore be represented at the level of the discrete source as

$$\mathbf{F}(\mathbf{k}; \chi) = \cos \chi \mathbf{F}^{sc}(\mathbf{k}) + \sin \chi \mathbf{F}^{ed}(\mathbf{k}),$$

and the vertex entering the memory kernel is

$$V_\alpha(\mathbf{k}; \chi) = \mathbf{e}_\alpha(\mathbf{k}) \cdot \mathbf{F}(\mathbf{k}; \chi),$$

with $\mathbf{e}_\alpha(\mathbf{k})$ the phonon polarization vectors.

For the high-symmetry directions considered here, each branch α is either polarised parallel to $\mathbf{t}$ or perpendicular to it. Modes with $\mathbf{e}_\alpha \parallel \mathbf{t}$ couple only to $\mathbf{F}^{sc}$, whereas modes with $\mathbf{e}_\alpha \perp \mathbf{t}$ couple only to $\mathbf{F}^{ed}$. It follows that the mixed vertex has no branchwise interference term,

$$|V_\alpha(\mathbf{k}; \chi)|^2 = \cos^2 \chi |V_\alpha^{sc}(\mathbf{k})|^2 + \sin^2 \chi |V_\alpha^{ed}(\mathbf{k})|^2,$$

and the radiated power separates into an affine combination

$$P(\chi) = \cos^2 \chi P_{sc} + \sin^2 \chi P_{ed},$$

with P_{sc} and P_{ed} the screw and edge powers computed in Sec. VIII. In the velocity ranges where the mobility is dominated by viscous radiative drag this translates directly into

$$B(\chi) \simeq B_{sc} \cos^2 \chi + B_{ed} \sin^2 \chi,$$

which is consistent with molecular dynamics observations for mixed dislocations in cubic metals. Beyond the high-symmetry configurations considered here, one expects small corrections to this simple interpolation when the block structure of the dynamical matrix is relaxed or when additional damping channels are included; these will be the subject of future work.

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- $$P_{\max} \sim \frac{\mu B^2}{c_T^2} \frac{k_0^3 a^3}{(2\pi)^3} \omega_D, \quad (179)$$
- where we have included the Debye frequency $\omega_D \sim c_T k_0$ as the characteristic emission frequency. With $k_0 = \pi/a$, this yields:
- $$P_{\max} \sim \frac{\mu B^2 c_T}{8a}. \quad (180)$$
- The stress required to sustain motion at $v_d = c_L$ follows from the power balance $\tau B c_L = P_{\max}$:
- $$\tau_{\text{supersonic}} \sim \frac{\mu B c_T}{8a c_L}. \quad (181)$$
- For typical metals where $c_L \approx 2c_T$ and $B = b \approx a/\sqrt{2}$ (fcc), we obtain:
- $$\tau_{\text{supersonic}} \sim \frac{\mu}{16\sqrt{2}} \approx \frac{\mu}{23}. \quad (182)$$
- Comparing to the ideal shear strength $\tau_{\text{ideal}} \approx \mu/18$, this suggests that supersonic motion requires stresses approaching 30%–80% of the ideal strength. Given that real crystals typically fail through nucleation of defects or cracks at $\sim 0.1\tau_{\text{ideal}}$, sustained supersonic dislocation motion appears unlikely in practice. However, transient supersonic motion following high-velocity nucleation events or shock loading remains kinematically possible, as observed in molecular dynamics simulations [62,64].
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